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EVALUATION OF THE ENERGY TRANSFER  
IN THE CHAR ZONE DURING ABLATION

Part II: In-Depth Response of Ablative Composites

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IN DEPTH RESPONSE OF  
ABLATIVE COMPOSITES

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by

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May 1975

## PREFACE

This report is the second of two parts and completes the documentation on NASA Grant NGR-19-001-015. It also served as the PhD dissertation for Edwards G. del Valle.

APPENDIX A

EXPLANATION OF THE COMPUTER IMPLEMENTED SOLUTIONS OF  
THE ENERGY TRANSFER FOR DECOMPOSITION  
IN-DEPTH OF PLASTIC ABLATORS

The ABLATIN1 and ABLATIN2 systems are general analyses implemented in FORTRAN IV for studying the energy transfer in the combined decomposition/char zone of a charring ablator. Both of these analyses treat the decomposition of the virgin material in the same fashion. Namely, a pseudo-order kinetic expression of the form of Equation (2-1) is used to describe the decomposition process. These analyses differ, however, in the way the chemical generation term is calculated in the char zone. As was explained in Chapter III, there are three chemically distinct flow conditions that are considered, which are, frozen, equilibrium and non-equilibrium flow. The ABLATIN1 analysis considers the pyrolysis gases to be either frozen (not chemical reactions) or, in chemical equilibrium. The frozen flow and equilibrium flow cases give the lower and upper limits of the total energy transfer in the decomposition-char zone, respectively. The ABLATIN2 analysis considers only the gases to be in chemical non-equilibrium: i.e., the rate of reaction is described using finite rate chemistry. Both analyses require that the temperature, the heat flux and the composition



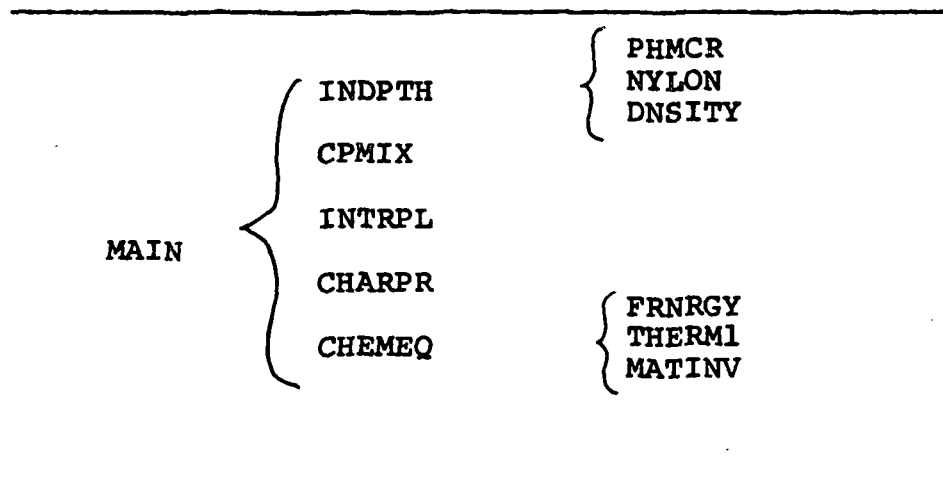
of the pyrolysis gases be specified. Unfortunately, as was said in Chapter III, the current state of the art precludes prediction of the composition of the pyrolysis products from a known combination of plastic composites and therefore it was necessary to specify the pyrolysis gas composition. The boundary conditions selected are written in Equation (3-27).

Once the energy equation is solved, the momentum equation is solved by specifying the front surface pressure. Because the pressure drop is small ( $\sim 15$  lbs/ft<sup>2</sup>), compared to the total pressure ( $\sim 2160$  lbs/ft<sup>2</sup>), the assumption of constant pressure in the solution of the energy equation can be considered valid and the equations can be uncoupled. In both analyses the surface recession velocity is specified and the mass flux of pyrolysis gases is calculated from Equation (3-1). Furthermore, the analyses do not require the arbitrary specification of a char thickness, which is calculated.

#### The ABLATIN1 System

This analysis provides the lower and upper limits of the total energy transfer in the combined decomposition-char zone by considering the pyrolysis gases to be in frozen, or in chemical equilibrium. This analysis consists of a MAIN program and eleven subroutines. Two of these subroutines are major subroutines in the sense that they control the flow of information to other minor subroutines. A hierarchical diagram of this is shown in Figure A-1. The two major sub-

Figure A-1. Hierarchical System  
Diagram of ABLATIN1



routines are INDPATH and CHEMEQ and their functions are explained below. The MAIN program has direct access to three other subroutines, which are, CPMIX, INTRPL, and CHARPR. An explanation of each subroutine follows next.

INDPTH: This is one of the two major subroutines. In it the physical properties of the virgin material as a function of temperature are calculated. The thermal conductivity gradient is likewise calculated in this subroutine for use in the general energy equation. In addition, the energy absorbed ( $\text{BTU/FT}^3\text{-sec}$ ) due to the degradation of the plastic composites is calculated using the information generated by three minor subroutines, which are: PHMCR, NYLON, and DNSITY. The functions of each one of these subroutines are subsequently explained.

PHMCR: In this subroutine the heat absorbed by the degradation of phenolic resin and phenolic-microballoons is calculated based on the data of Sykes and Nelson (1). The heat term has the units of BTU/lb of each composite.

NYLON: Similar in nature to PHMCR, this subroutine calculates the heat absorbed (in BTU/lb) due to the degradation of nylon based also on the data of Sykes and Nelson (1).

DNSITY: This subroutine calculates the rate of density change of each individual composite (i.e., nylon, phenolic and phenolic-microballoons), which provides the information required to compute the mass flux of pyrolysis gases. In addition, this subroutine is used to control the Runge-Kutta step size while the solution of the energy equation is

marching through the decomposition zone. The density changed (in  $\text{lbs/ft}^3\text{-sec}$ ) calculated in this subroutine along with the heat (in  $\text{BTU/lb}$ ) calculated in PHMCR and NYLON are used to generate the  $q(T)$  term (in  $\text{BTU/ft}^3\text{-sec}$ ) in the general energy equation. (See Equation (3-20)). The calculation of  $q(T)$  is performed in subroutine INDPATH.

The first four subroutines just described, PHMCR, NYLON, INDPATH, and DNSITY, constitute the principal subroutines used in describing the physico-chemical changes of the decomposition of nylon-phenolic resin composites. These four subroutines are used when the numerical solution is marching along the decomposition zone. When the decomposition of the virgin material is complete, that is, the virgin material has degraded to gases and char residue, the program has two options. One is to describe the gases with a frozen flow chemistry, in which case the composition of the gases stay constant with temperature, or, to describe the gases with an equilibrium chemistry, in which case the composition of the gases change with temperature and are computed from thermodynamic principles. Both options are explained below.

Frozen Flow Analyses: Under this option the energy equation is solved assuming that there are no chemical reactions taking place in the char zone and hence the chemical composition of the gas mixture does not change. This method of analysis gives the lower bound of the energy absorbed within the char zone. It is the simplest, in terms of numerical solution and the fastest to solve on a machine,

requiring about one minute on an IBM 360/65 computer. Under this option two subroutines are called, these are: CPMIX and CHARPR. An explanation of their functions follows.

CPMIX: This subroutine is called by MAIN to calculate the average heat capacity of a frozen flow mixture. This subroutine is called at every new temperature generated by the Runge-Kutta analysis. The heat capacity of each individual specie is generated by an empirical fit which is read in by MAIN. The thermodynamic data used is given in Appendix C.

CHARPR: The data of Southern Research Institute (2) is used in this subroutine to generate the thermal conductivity, the thermal conductivity gradient and the heat capacity of the char as a function of temperature. Unlike CPMIX, this subroutine is also used by the chemical equilibrium analysis option. The actual data used is presented in Appendix C.

Equilibrium Flow Analysis: This analysis is the second option of the ABLATIN1 system to describe the chemistry in the char zone. The primary difference with the frozen flow analysis is that the equilibrium analysis accounts for concentration changes due to chemical reactions, which are assumed to be in thermodynamic equilibrium. A free energy minimization technique is used to compute the equilibrium composition as a function of temperature. This technique was developed in Chapter IV and the reader is referred to this Chapter for further details. The Equilibrium Flow Analysis uses in addition to CHARPR, five other subroutines which are:

CHEMEQ, which minimizes the free energy; FRNGY, which calculates the free energy function to be minimized; MATINV which inverts the matrix and solves the simultaneous linear equations; THERM1, whose primary function is to calculate the heats of formation of the chemical species; and INTRPL which is used to interpolate the values generated by CHEMEQ and which are needed for the solution of the general energy equation. A more complete explanation of the functions of each subroutine follows next.

CHEMEQ: This is the other major subroutine. This subroutine is called by MAIN when the marching procedure is in the char zone. In this subprogram the equilibrium composition of a multi-component, polyphase system is calculated using free energy minimization technique, which has been explained in Chapter IV. This subroutine is called once throughout the analysis. The equilibrium compositions of each individual species are computed and stored as functions of temperature. In addition, the mass flux, the average molecular weight, the average heat capacity of the mixture and the heat absorbed due to chemical reactions are also stored as functions of temperature. All of these stored values are later used to generate interpolated values needed in the solution of the general energy equation.

To verify the calculations made by this program, several literature examples were used for comparison and the reader is referred to Chapter IV for these comparisons.

FRNGY: This subroutine supplies the free energy func-



tion to be minimized by CHEMEQ. This subroutine is called at every temperature at which an equilibrium composition calculation is performed. In addition, the heat capacity of each individual species is also calculated.

MATINV: This subroutine is a standard method for solving a set of linear equations by inverting a non-singular  $n \times n$  matrix. The inversion is performed iteratively by reducing the original matrix to an identity matrix by a series of row operations. The method is then repeated with the resulting identity matrix. The IBM Share Library is the source for this particular program (3). The simultaneous solution of the linear equations (see Table 4-1) gives the Lagrange multipliers which are used to generate the new composition of the gases for the next iteration (see Equation (4-32)). In addition, when there are solid species, the solution of the linearized equations (see Table 4-1) results in the explicit computation of the number of moles of these species directly. This is not the case for the gas species.

THERM1: The calculation of the heat of formation and the entropy of each chemical species is performed in this subroutine. This subroutine is called by CHEMEQ after the species compositions are calculated. The reference temperature used in the calculations is  $298.16^\circ\text{K}$ .

INTRPL: This is a general purpose Lagrangian interpolation subprogram with non-equal step size between points. This subprogram is used by MAIN to interpolate the stored values generated by CHEMEQ. In addition, INTRPL is used in

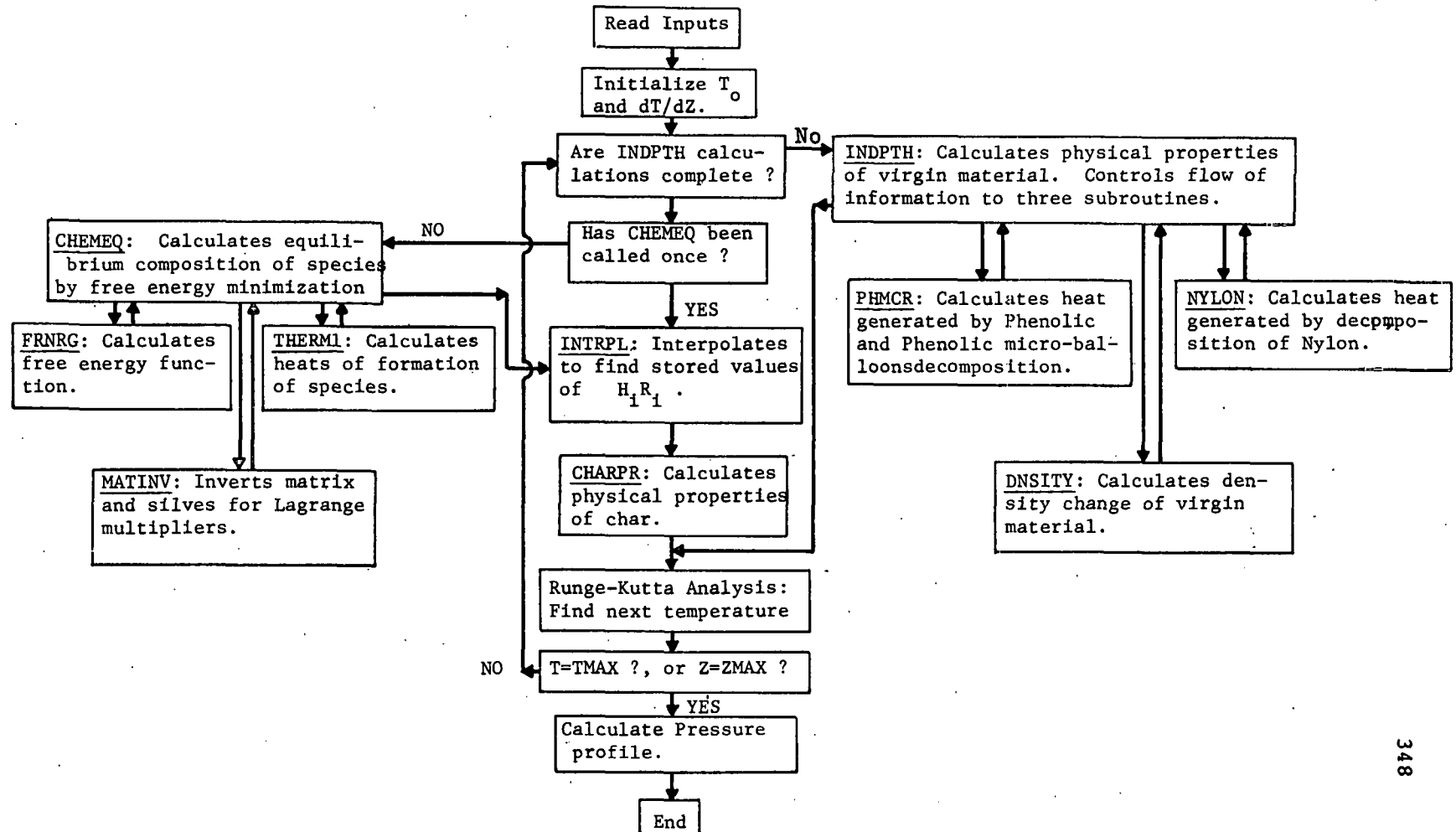
the solution of the uncoupled momentum equation to interpolate values generated during the solution of the energy equation.

The five subroutines just mentioned in addition to CHARPR, constitute the principal subroutines used in describing the physico-chemical changes which occur within the char zone.

Next a brief description of MAIN (the main program) follows. In it the calling sequence of the subroutines for the chemical equilibrium analysis option and the frozen flow analysis are explained.

MAIN: The main program solves the energy equation by using a Runge-Kutta formulae of the form developed in Chapter III. MAIN is assisted in the solution of the energy equation by ten subroutines for the equilibrium analysis, and by two subroutines for frozen flow analysis. As was explained, CHARPR is used by both analyses, so that the total number of subroutines is eleven. A block flow diagram of the main program for the chemical equilibrium option is shown in Figure A-2. After the data is read in and variables are initialized MAIN proceeds to call subroutine INDPTH to generate the physico-chemical properties for the decomposition process. INDPTH interacts with PHMCR, NYLON and DNSITY to obtain the mass flux, heat of reaction and other variables as was previously explained. Once these properties have been calculated MAIN proceeds to calculate the next temperature point in the Runge-Kutta analysis.

Figure A-2. Block Flow Diagram of the ABLATIN1 Program.



This operation is repeated until the virgin material has been totally degraded to gases and char. At this instance MAIN calls CHEMEQ to generate the equilibrium composition of the reacting gases, along with other needed information such as: mass flux of the gases, average molecular weight, the average heat capacity of the mixture and the heat absorbed due to chemical reactions. Unlike subroutine INDPATH, which was called at every new temperature, subroutine CHEMEQ is called only once. This can be done because the equilibrium composition is only a function of temperature and pressure. Pressure is assumed constant through the analysis, and the equilibrium composition, the mass flux, the average molecular weight, the average heat capacity of the mixture and the heat absorbed due to chemical reactions are stored as functions of temperature. Since every new temperature generated by the Runge-Kutta analysis does not coincide with the temperature of the stored information, an interpolation scheme is necessary to generate these values at these intermediate temperatures. This interpolation function is performed by subroutine INTRPL. It was found by this author that storing the equilibrium composition every 10°K was sufficient to give accurate interpolated values at intermediate temperature points. After the interpolation is performed CHARPR is called to generate the physical properties for the char. A new temperature is then generated and the procedure is repeated until the temperature of the char reaches the sublimation temperature of carbon at the given

pressure.

For frozen flow the numerical solution while in the decomposition zone is the same. When the marching solution enters the char the primary difference is that CHEMEQ and INTRPL subroutines are bypassed. Instead, MAIN calls CPMIX to generate the heat capacity of the frozen flow mixture and then proceeds to call CHARPR for the physical properties of the char. A new temperature is generated as in the equilibrium case and the process is repeated until the temperature of the char reaches the sublimation temperature of carbon at the given pressure.

Once the temperature profile is established, i.e., the energy equation has been solved, the program proceeds to calculate the pressure profile. More is said about the pressure calculations after the description of the ABLATIN2 System which follows below.

### The ABLATIN2 System

This analysis is programmed exclusively for non-equilibrium flow chemistry where the rate of reaction of each species is described by finite rate chemistry. Compared to the chemical equilibrium analysis, the non-equilibrium flow analysis is easy to program. It takes three DO LOOPS and about 20 FORTRAN statements to calculate the rate of reaction of a chemical species which is simultaneously reacting in more than one chemical reaction.

The computing time for the non-equilibrium analysis

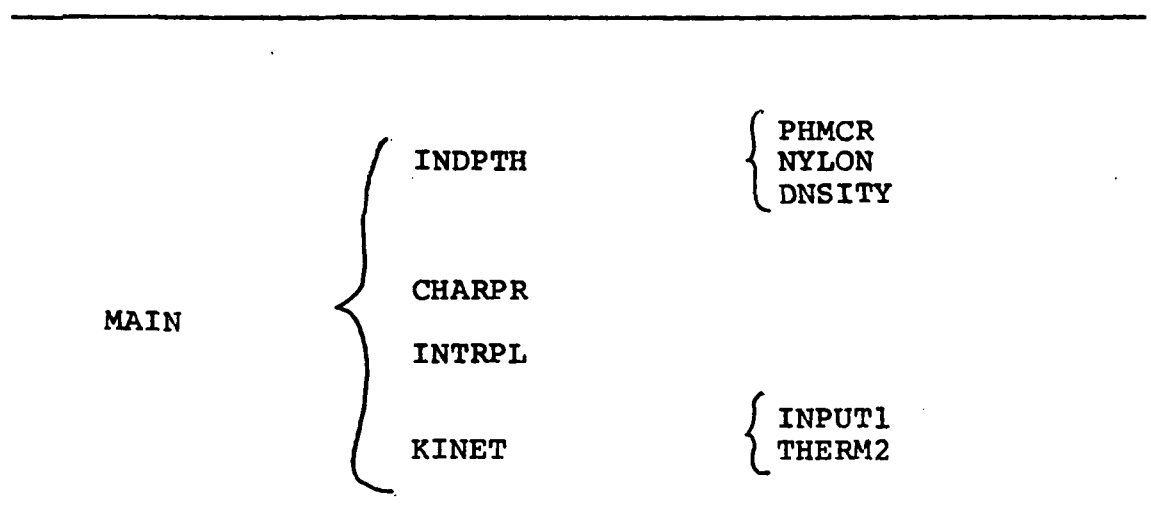
however, exceeds that of chemical equilibrium by a factor of about 10. As was explained in Chapter V, this is due in part to the stiffness of the general energy equation caused by very fast chemical reactions taking place in the flow field. This stiffness requires that the step size be of the order of  $10^{-7}$  to  $10^{-8}$  feet to maintain numerical stability. Because the step size was so small many operations had to be made double precision to reduce round-off error. Operations in double precision arithmetic also increased the computing time.

In comparing Figure A-1 and Figure A-3 it is seen that the ABLATIN1 and ABLATIN2 systems use the same subroutines to describe the decomposition process. These subroutines are: INDPATH, PHMCR, NYLON and DNSITY. In addition, CHARPR and INTRPL and the four previously mentioned subroutines perform the same functions in both the ABLATIN1 and ABLATIN2 systems and will not be described again.

Non-Equilibrium Flow Analysis: The primary difference between the equilibrium and non-equilibrium flow analyses is the way the rate of production of chemical species is computed. In the chemical equilibrium analysis the rate of production of species, is computed from thermodynamic principles, while for non-equilibrium, finite rate chemistry is used. The rate of reaction of each species is computed by subroutine KINET. In the non-equilibrium flow analysis, changes in the mole flux of each species with temperature must be calculated as part of the Runge-Kutta analysis. That



Figure A-3 Hierarchical System  
Diagram of ABLATIN2



is, for each temperature generated in the Runge-Kutta analysis, a corresponding set of concentrations must be calculated. This requires that KINET be called by MAIN at every new increment of temperature. This is necessary because the concentration changes are not only functions of temperature and pressure, but of composition as well. KINET in addition calls two other subroutines, INPUT1 and THERM2 and their functions are subsequently explained.

KINET: This subprogram is the counterpart of CHEMEQ. In it the reaction rate of each species is computed using finite rate data read in by INPUT1. The mole fraction, the total mass flux, the average molecular weight, the heat capacity of the mixture and the heat absorbed due to chemical reactions are also computed and stored for later use in the calculations. In addition, this subroutine controls the step size of the Runge-Kutta analysis to maintain stability. For the CHEMEQ analysis the step size needed to maintain stability is of the order of  $10^{-4}$  to  $10^{-5}$  feet, while for KINET a step size of the order of  $10^{-7}$  to  $10^{-8}$  feet is necessary to maintain stability in regions where rapid chemical changes are occurring.

INPUT1: This subroutine reads in the kinetic data needed to compute finite rate chemistry.

THERM2: This subprogram is similar to THERM1 with the difference that the heat capacity of each species is calculated in addition to the heats of formation. This subprogram is called by KINET at every temperature.

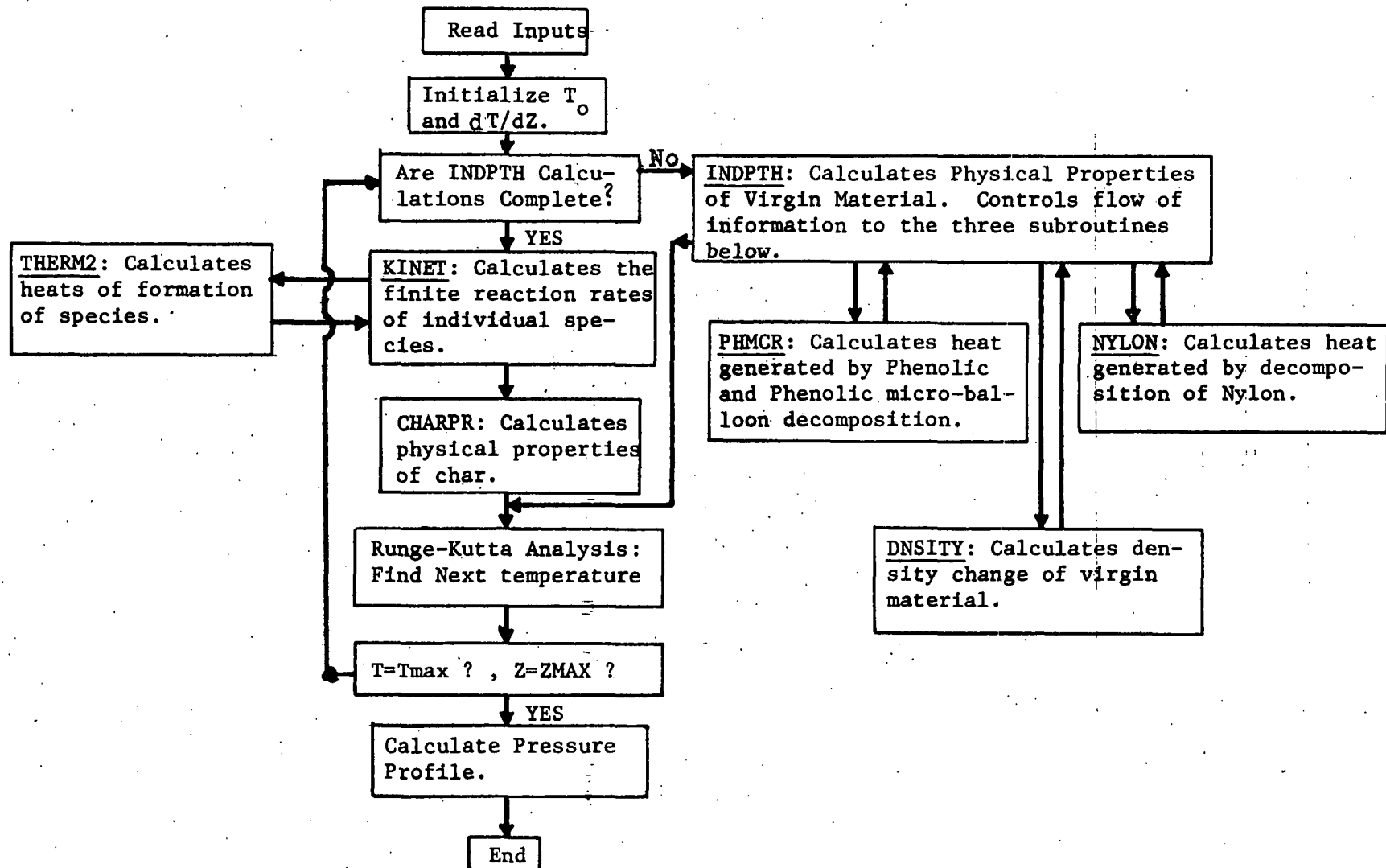
MAIN: The main program of ABLATIN2 performs very similar operations as that for the ABLATIN1 system. In Figure A-4 a block flow diagram of the ABLATIN2 system is given. The principal difference is that in ABLATIN1, MAIN calls CHEMEQ to generate the compositions of the species while in this case KINET is called by MAIN. The rest of the computations are the same as has been explained before.

### Calculation of the Pressure Distribution

The pressure distribution through the char zone is calculated by integrating Equation (3-13) using a Simpson's rule integration. Since it was shown in Chapter III that this equation could be uncoupled from the energy equation, its solution is calculated after the temperature distribution is known. Therefore, the integration method for this momentum equation is the same for both the ABLATIN1 and ABLATIN2 system. Interpolation using subprogram INTRPL of both char distance and collision integral as a function of the temperature distribution across the char is required. These operations allow the calculation of the gas mixture viscosity as a function of char distance. The pressure calculation scheme used in this research was developed by April (4).

Simpson's Rule Integration Step: As discussed in Chapter III, the Simpson's Rule formula is used to integrate the pressure equation, Equation (3-13). As with the Runge-Kutta analysis it is necessary to select a step size that gives a fast, yet accurate solution to the equation. April

Figure A-4. Block Flow Diagram of the ABLATIN Program.



(4) made a study of several interval sizes and his results are presented in Table A-1. As noted in this table, April (4) found that the solution of the momentum equation becomes stable with twenty integration steps.

### Summary

In this appendix an introduction to the ABLATIN1 and ABLATIN2 systems was given. The ABLATIN1 system was developed to compute the total energy absorbed in the combined decomposition-char zone for a frozen and equilibrium flow model. These two analyses gave the lower and upper limits of the energy absorbed within the combined zones. The ABLATIN2 analysis was developed exclusively for non-equilibrium flow chemistry. This analysis was said to be more time consuming on a computing machine, although it is simpler to program than the other two models. The various functions of each subprogram was explained in detail and block flow diagrams for both the ABLATIN1 and ABLATIN2 systems were given. Finally, a brief explanation on the solution of the pressure equation by MAIN, was given.

In Appendix B a complete listing of the ABLATIN1 and ABLATIN2 systems is presented along with typical input and output data for the frozen, equilibrium and non-equilibrium flow chemistry.

TABLE A-1:

Comparison of Various Simpson's Rule Increment  
 Sizes for the Frozen Flow, Variable Physical  
 Properties Analysis After April (4).

Dimensionless Char Distance (Z/L)	Pressure (lb/ft <sup>2</sup> ) Simpson's Rule Increment Size			
	20	50	100	200
0.00	2175.5921	2175.5918	2175.5913	2175.5912
0.33	2173.4147	2173.4144	2173.4139	2173.4138
0.67	2168.7373	2168.7368	2168.7364	2168.7364
1.00	2160.0000	2160.0000	2160.0000	2160.0000

Conditions:  $W = 0.05 \text{ lb/ft}^2\text{-sec}$        $L = 0.0208 \text{ ft}$        $\xi = 0.8$

Gas Composition (Mole/Mole Gas):

$\text{CO} = 0.245$ ,  $\text{CO}_2 = 0.046$ ,  $\text{N}_2 = 0.073$ ,  $\text{CH}_4 = 0.570$ ,  $\text{C}_6\text{H}_6 = 0.068$



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1. Sykes, G. F., and J. B. Nelson, "Thermodynamic of Ablation Materials", Preprint 7B, 61st National Meeting, AIChE, Houston, Texas (Feb. 19-23, 1967).
2. Engelke, W. T., C. M. Pyron, Jr., and C. D. Pears, "Thermophysical Properties of a Low Density Phenolic Nylon Ablation Material". NASA CR-809 (July, 1967).
3. Sadaka, R. N., "Double Precision Matrix Inversion with Selective Pivot", IBM Share Library No. 7090-fl, B181 INV2(1965).
4. April, G. C., "Evaluation of the Energy Transfer in the Char Zone During Ablation", PhD. Dissertation, Louisiana State University, Baton Rouge, May 1969.

## APPENDIX B

### THE ABLATIN1 AND ABLATIN2 ANALYSES

As discussed in Appendix A, the ABLATIN1 and ABLATIN2 programs are general analyses implemented in FORTRAN IV for studying the energy transfer in the decomposition zone and char zone of char forming ablators. The ABLATIN1 analysis was said to consider the pyrolysis gases to be either frozen, or in chemical equilibrium. The ABLATIN2 analysis on the other hand, considers the gases to be in chemical non-equilibrium.

As was shown in Appendix A a great degree of overlap exists in the many common subroutines used by the two analyses. The rationale, however, for keeping the ABLATIN1 and ABLATIN2 analyses as separate programs was due to core restrictions. There were, in addition, other practical considerations regarding input-output which made the separate development of these programs more practical.

A listing of the ABLATIN1 program with all the subroutines is presented in Table B-1. An explanation of the function of each subroutine has been given in Appendix A. Most of the subroutines are self-explanatory with most of the major functions explained through comment cards. The degree of modularity of this program makes it highly flexible, and subject to easy modification in the future. For this reason the author has provided an extensive nomenclature of every

important variable in the program. This was done in the hope of minimizing errors incurred in modifying any subroutine. Furthermore, the listing allows easy cross referencing of variables among subroutines, which will further reduce the possibility of errors.

Communication among subroutines is mostly done by means of labeled common blocks, thus minimizing communication through arguments of a call. This was done to reduce computer time among frequently called subroutines. However, this method of structuring communication can be very error prone and was an additional motivation for providing a nomenclature listing of every important variable. In this way any modification of a variable can be cross checked in the nomenclature listing of every subroutine. A detailed explanation of the input format is also given in this Appendix.

Following the listing and explanation of input format for the ABLATIN1 program, is the listing of ABLATIN2. The ABLATIN2 is listed in Table B-4. In both cases, typical input data and output results are listed.

TABLE B-1. Listing of ABLATINI Program

C		1
C		2
C		3
C	-----INDEPTH RESPONSE OF AN ABLATIVE COMPOSITE	4
C	EQUILIBRIUM ANALYSIS.	5
C	ABLATINI SYSTEM	6
C		7
C		8
C		9
C		10
	COMMON/KA/S1(6),S2(6),S3(6),S4(6),S5(6),S6(6),A11(6),	11
	1A22(6),A33(6),A44(6),A55(6),A66(6),AA(30,6),JCODE(6)	12
	COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),FI(30),	13
	1GI(30),AII(30),BII(30),CII(30),DII(30),EII(30),	14
	2FII(30),GII(30),TLOW(30)	15
	COMMON/KC/ICODE(30),Y(30),FW(30)	16
	COMMON/KCC/SPCIE1(30),SPCIE2(30),TABLE(353,25)	17
	COMMON/KE/XTKE(100),ZOMGA(100),EK(100),SIG(100)	18
	COMMON/KEE/PL,RR,TZERO,EPS,KEY,NN,NQ,MM	19
	COMMON/KI/W,KMAX,KOUNT	20
	COMMON/KJ/DELTK,TVAR	21
	COMMON/KF/CPS,CDO,DCDO,JCHAR,TC	22
	COMMON/KK/IP	23
	COMMON/KL/WTOTAL,RHOII	24
	COMMON/KM/XMOL(30)	25
	COMMON/KNN/TFMAX	26
C		27
C		28
C		29
	DIMENSION TOK(200),CHARDN(200),Z1(200),T1(200),ZX(41),ZY(41),	30
1	TP(41),P(41),WFLUX(41),TT(21),PROD(21),	31
	2YCOMP(30,41),PRODCP(21),PRODR(21),COND(30),CV(30),	32
	3VIS(30),YI(30)	33
C		34

C		35
	DOUBLE PRECISION ZZ,H11,ZLL,TTTT,DTCC	36
C		37
C		38
C		39
C	-----DEFINE THE ARITHMETIC STATEMENT FUNCTIONS FOR THE	40
C	RUNGE-KUTTA ANALYSIS.	41
C		42
C		43
	F(A)=+GROUP*A	44
	G(A)=A	45
C		46
C		47
C		48
C		49
C	RR=GAS CONSTANT(1.98726BTU/(LB-MOLE OR)	50
C	TZERO=REFERENCE TEMPERATURE	51
C	TFMAX=MAXIMUM ALLOWABLE TEMPERATURE FOR THIS MODEL (OF)	52
C		53
	RR=1.98726	54
C		55
C		56
C	HSIMPI=SIMPSON'S RULE INCREMENT SIZE(FT) USED	57
C	IN THE SOLUTION OF THE MOMENTUM EQUATION	58
C		59
	FR2=778.16/32.2	60
C		61
C		62
C	NC=NO. OF GAS SPECIES	63
C	NNS=NO. OF LIQUID OR SOLID SPECIES	64
C	NS=NC+NNS(TOTAL NUMBER OF SPECIES)	65
C	MM=NO. OF ELEMENTS	66
C	KODE=1 CONDUCTIVITY OF CHAR WITH GAS IN PORES	67
C	KODE=2 CONDUCTIVITY OF CHAR WITH PORES EVACUATED	68

C	KEY=1(FROZEN),=2(EQUILIBRIUM)=3(NON-EQUILIBRIUM)	69
C	PL=PRESSURE AT Z=L(LB/FT2)	70
C	DELTK=TEMPERATURE INCREMENT	71
C	TO=TEMPERATURE AT Z=0	72
C	EPS=CHAR POROSITY	73
C	ZL=ABLATOR THICKNESS(IN FEET)	74
C	HI=INITIAL RUNGE-KUTTA INCREMENT SIZE(FT) USED	75
C	IN THE SOLUTION OF THE ENERGY EQUATION.	76
C	ALPHA=VISCOUS COEFFICIENT IN DARCY'S EQUATION(1/FT)	77
C	BETA=INERTIAL COEFFICIENT IN DARCY'S EQUATION(1/FT2)	78
C	SIGMA=STEPHAN-BOLTZMAN CONSTANT(0.481X10-12 BTU/FT2-SEC-OF4)	79
C	EMIS=CHAR EMISIVITY.	80
C	QFLUXI=INITIAL BACK SURFACE HEAT FLUX.	81
C	TCHAR=BACK SURFACE TEMPERATURE OF CHAR	82
C		83
C		84
	FR=0.1666667	85
C		86
C		87
C	-----READ INPUT PARAMETERS	88
C		89
C		90
10	READ11,NC,NNS,MM,KODE,KEY	91
11	FORMAT(6I6)	92
12	FORMAT(F10.3,10X,5F10.3)	93
	READ 12,PL,TO,EPS,ZL,HI,TFMAX	94
	READ21,ALPHA,BETA,SIGMA,EMIS	95
	READ13,DTC,TCHAR,VR	96
13	FORMAT(7E10.3)	97
	NN=NC	98
	NS=NC+NNS	99
	NQ=NS	100
	QFLUX=QFLUXI	101
C		102



C		103
C	S1...S6(APPLY BETWEEN 1000-6000 OK)	104
C	A11...A66(APPLY BETWEEN 300-1000 OK)	105
C	JCODE(J)=0 THE REFERENCE ELEMENT IS IN THE GAS STATE.	106
C	JCODE(J)=1 THE REFERENCE ELEMENT IS IN THE SOLID STATE.	107
C	AI...EI(HEAT CAPACITY CONSTANTS...1000-6000 OK)	108
C	FI,GI(NEEDED TO CALCULATE THE ENTHALPY,ENTROPY	109
C	AND FREE ENERGY....1000-6000 OK)	110
C	AII...GII(300-1000 OK)	111
C	AA=FORMULA NUMBER. GIVES THE ATOMS OF ELEMENT J	112
C	IN SPECIE I.	113
C		114
C	TLOW(I)=MINIMUM TEMPERATURE AT WHICH THE HIGH TEMPERATURE	115
C	FIT IS APPLICABLE.	116
C	FW(I)=MOLECULAR WEIGHT OF SPECIE I.	117
C	YI(I)=MOLE FRACTION OF SPECIE I.	118
C	SPCIE1 AND SPCIE2 ARE THE SPECIES IDENTIFICATION	119
C	ICODE(I)=0 SPECIE IS A GAS	120
C	ICODE(I)=1 SPECIE IS A SOLID	121
C		122
C		123
C		124
C		125
C	-----READ EMPIRICAL CONSTANTS TO CALCULATE THE SENSIBLE	126
C	ENTHALPY CHANGE OF THE CONSTITUENT ELEMENTS.	127
C		128
C		129
	DO 9 J=1,MM	130
	READ 18,S1(J),S2(J),S3(J),S4(J),S5(J),S6(J),JCODE(J)	131
	READ 18,A11(J),A22(J),A33(J),A44(J),A55(J),A66(J)	132
9	CONTINUE	133
	DO15I=1,NS	134
	READ 14,TLOW(I),FW(I),YI(I),SPCIE1(I),SPCIE2(I),ICODE(I)	135
14	FORMAT(10X,3E10.3,2X,2A3,I4)	136

C		137
C		138
C	-----READ EMPIRICAL CONSTANTS TO CALCULATE THE HEAT	139
C	CAPACITY OF THE SOLID PLUS TWO ADDITIONAL CONSTANTS	140
C	TO CALCULATE THE ENTHALPY, THE ENTROPY AND THE FREE	141
C	ENERGY OF THE SYSTEM	142
C		143
C		144
	READ13,AI(I),BI(I),CI(I),DI(I),EI(I),FI(I),GI(I)	145
	READ13,AII(I),BII(I),CII(I),DII(I),EII(I),FII(I),GII(I)	146
C		147
C		148
C	-----READ IN THE FORMULA NUMBERS	149
C		150
C		151
15	READ13,(AA(I,J),J=1,MM)	152
C		153
C		154
C		155
C	EK=POTENTIAL PARAMETER/BOLTZMAN CONSTANT.	156
C	SIG=COLLISION DIAMETER(ANGSTRONG UNITS).	157
C	THESE CONSTANTS ARE USED TO DETERMINE THE	158
C	VISCOCITY AND THERMAL CONDUCTIVITY OF THE	159
C	REACTING GAS MIXTURE.	160
C		161
C	NDATA=NO. OF XTKE VS. ZOMGA DATA POINTS	162
C	XTKE=PRODUCT OF TEMPERATURE AND 1/EK VALUE	163
C	ZOMGA=COLLISION INTEGRAL TABULATED VS XTKE	164
C		165
C		166
C		167
	READ16,(EK(I),SIG(I),I=1,NC)	168
16	FORMAT(2F15.5)	169
	READ11,NDATA	170

READ17,(XTKE(I),ZOMGA(I),I=1,NDATA)	171
17 FORMAT(2F15.5)	172
18 FORMAT(6E10.4,I3)	173
21 FORMAT(3E15.5,F15.5)	174
C	175
C	176
C	177
C-----INITIALIZATION OF PARAMETERS	178
C	179
C	180
C	181
C N=COUNTER OF RUNGE KUTTA STEPS	182
C	183
C N=1	184
C	185
C TO=INITIAL TEMPERATURE OF BACK SURFACE(OF)	186
C IT IS A SPECIFIED BOUNDARY CONDITION.	187
C TC=TO	188
C	189
C TC=INSTANTANEOUS TEMPERATURE OF THE SYSTEM(OF)	190
C	191
C K1=1	192
C	193
C-----K1=GIVES THE TOTAL NUMBER OF DATA POINTS STORED.	194
C SHOULD NOT EXCEED THE DIMENSION OF VARIABLES.	195
C	196
C KOUNT=1	197
C	198
C	199
C-----KOUNT IS A CODE. IT IS USED TO DETERMINE WHETHER	200
C THE CHEMEQ SUBROUTINE SHOULD BE CALLED OR BYPASSED.	201
C THE LOGIC IN THIS PROGRAM IS SUCH THAT CHEMEQ IS	202
C CALLED ONLY ONCE. THIS IS POSSIBLE BECAUSE AT EQUILIBRIUM	203
C THE COMPOSITION IS ONLY A FUNCTION OF TEMPERATURE AND	204

C	PRESSURE AND NOT A FUNCTION OF RESIDENCE TIME AS IS IN	205
C	THE KINETICS CASE. WHEN KOUNT=2 CHEMEQ IS BYPASSED.	206
C		207
	ROCHAR=13.	208
	TZERO=298.159	209
	K1=0	210
	IND=0	211
	K10=0	212
	DELTF=0.	213
C		214
	REAC1=0.	215
C	REAC1=RATE OF HEAT ABSORBED BY THE CHEMICAL REACTIONS IN	216
C	(BTU/FT**2-SEC)	217
C		218
C		219
	CPB1=0.	220
C	CPB1=RATE OF HEAT ABSORBED BY THE FLOWING GASES IN	221
C	(BTU/FT**2-SEC)	222
C		223
C		224
	CPB2=0.	225
C	CPB2=RATE OF HEAT ABSORBED BY THE SOLIDS(BTU/FT**2-SEC)	226
C		227
	DCDOV=0.	228
	DCDO=0.	229
	DELTK=0.	230
C		231
C		232
C	-----NN5 GIVES THE NUMBER OF VARIABLES STORED IN TABLE(I,J).	233
C		234
C		235
	NN4=NC+5	236
	NN5=NN4+NNS	237
C		238

C	239
C	240
C-----THE FIRST FIVE VARIABLES ARE.....	241
C	242
C	243
C	244
C	245
C	246
C	247
C	248
C	249
C	250
C	251
C	252
C	253
C	254
C	255
C	256
C	257
C	258
C	259
C-----CALCULATE THE INITIAL AVERAGE MOLECULAR WEIGHT OF THE GAS	260
C	261
C	262
C	263
C	264
C	265
C	266
C	267
C	268
C	269
C	270
C	271
C	272

```

C
C
C-----THE FIRST FIVE VARIABLES ARE.....
C
C
C      1) THE TEMPERATURE(IN OK)
C      3) THE AVERAGE MOLECULAR WEIGHT
C      4) THE MASS FLUX(LBS/FT2-SEC)
C      2) THE HEAT TERM( UNITS? )
C      5) THE HEAT CAPACITY OF THE MIXTURE(CPMX)
C      6) THE REST OF THE VARIABLES ARE THE MOLE
C      FRACTIONS. FOR THE SOLIDS, THE TERM STORED
C      IS THE RATIO OF MOLES OF SOLID TO MOLE OF
C      GASES.
C
C
C      HI=INITIAL RUNGE-KUTTA STEP SIZE
C      H=HI
C
C
C
C-----CALCULATE THE INITIAL AVERAGE MOLECULAR WEIGHT OF THE GAS
C
C
C
C      SUMY=0.
C      DO 1 I=1,NN
C1     SUMY=SUMY+YI(I)
C      AVGFW=0.
C      DO31 I=1,NS
C      XMOL(I)=YI(I)/SUMY
C      Y(I)=YI(I)
C      IF(ICODE(I).EQ.1)GOTO31
C      AVGFW=AVGFW+Y(I)*FW(I)

```

31	CONTINUE	273
C		274
C		275
C	W=MASS FLUX(LBS/FT**2(TOTAL)-SEC)	276
	W=WI	277
C		278
C		279
C	-----THE UNITS OF MASS FLUX FOR THE PRESSURE PROFILE ARE:	280
	(LBS/FT**2(VOIDS)-SEC)	281
C		282
C		283
C		284
	Z=0.	285
C	Z=DISTANCE IN FEET	286
C	ZL=THICKNESS OF CHAR IN INCHES	287
C	ZINC=INCREMENTS OF DISTANCE AT WHICH VARIABLES	288
	SHOULD BE STORED.	289
C		290
C		291
	Z2=0.	292
C	Z2=VARIABLE USED TO COMPARE WHETHER THE DISTANCE	293
C	AT WHICH VARIABLES ARE STORED HAS BEEN REACHED.	294
C		295
C		296
	TVAR=(TC+459.69)/1.8	297
C	TVAR=TEMPERATURE IN OK.	298
C		299
	ZZ=0.	300
	ZLL=ZL/12.	301
	PRINT 51,ZLL,H	302
51	FORMAT(1X,'ZLL='D20.10,' H='E15.7)	303
C		304
C		305
C		306

C-----	INDEPTH RESPONSE OF ABLATIVE COMPOSITES.	307
C	FOR BACK SURFACE TEMPERATURE AND HEAT	308
C	FLUX SPECIFIED. THE EQUATION OF ENERGY	309
C	IS A SECOND ORDER, NON-LINEAR, ORDINARY DIFFERENTIAL	310
C	EQUATION WITH VARIABLE COEFFICIENTS.	311
C	THE NUMERICAL TECHNIQUE USED IS A 4TH ORDER	312
C	VARIABLE STEP RUNGE-KUTTA ANALYSIS.	313
C		314
C		315
C		316
C		317
C	TCHAR=TEMPERATURE AT WHICH ALL OF THE VIRGIN	318
C	MATERIAL HAS DECOMPOSED.	319
C		320
	ZINC=1.2E-5	321
	ZINC=2.2E-4	322
	DELZ=H	323
	H11=H	324
	IF(TVAR.GT.TCHAR)GOTO32	325
C		326
C		327
	CALL INDPH(TC,CDOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,	328
	1DELTK,N,DELZ,VR,W,H)	329
C		330
C		331
C		332
C	CDOV=THERMAL CONDUCTIVITY OF VIRGIN MATERIAL (	333
C	BTU/(FT-SEC-OF)	334
C	DCDOV=THE DERIVATIVE OF CDOV WITH TEMPERATURE(BTU/(FT-2EC))	335
C	GASCP=HEAT CAPACITY OF MIXTURE(BTU/LB-OF)	336
C	Q=HEAT ABSORBED BY DEPOLYMERIZATION OF THE	337
C	VIRGIN PLASTIC COMPOSITE(BTU/FT3-SEC)	338
C	CPV=HEAT CAPACITY OF VIRGIN COMPOSITE(BTU/LB-OF)	339
C	RHO=DENSITY OF VIRGIN COMPOSITE	340

C	DELTK=TEMPERATURE DIFFERENCE IN OK FOR A DISTANCE H.	341
C	N=NUMBER OF INTEGRATION STEPS	342
C	DELZ=INCREMENT OF DISTANCE(FT)	343
C	VR=SURFACE RECESSION VELOCITY(FT/SEC)	344
C	W=MASS FLUX(LBS/FT2-SEC)	345
C	H=RUNGE-KUTTA INTEGRATION STEP SIZE(FT)	346
C		347
C		348
	WI=W	349
C		350
	QCZI=CDOV*DTC	351
	DTCII=DTC	352
	PRINT 1390, QCZI	353
	1390 FORMAT(1X, 'QCZ='F15.5)	354
C		355
C		356
C	-----CALCULATE THE HEAT CAPACITY OF THE PYROLYSIS GASES	357
C		358
C		359
	CALL CPMIX(TVAR, NN, CPMX)	360
	GASCP=CPMX/AVGFW	361
	GOTO113	362
C		363
C		364
	32 CALL CHARPR	365
C		366
C		367
C		368
C		369
C	-----THIS SUBROUTINE CALCULATES THE THERMO-PHYSICAL	370
C	PROPERTIES OF THE CHAR	371
C		372
C		373
	DELZ=H	374



Z1(1)=0.	375
T1(1)=T0	376
ZLL=0.0208333	377
GOTO103.	378
101 TVAR=(TC+459.69)/1.8	379
IF(TVAR.GT.TCHAR)GOTO102	380
CALL INDPTH(TC,CDOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,DELTK,	381
IN,DELZ,VR,W,H)	382
C	383
C	384
C-----FOR EXPLANATION OF THE VARIABLES IN THE ARGUMENT SEE	385
C PREVIOUS CALL INDPTH STATEMENT.	386
C	387
C	388
C	389
C	390
C-----CALCULATE THE HEAT CAPACITY OF THE PYROLYSIS GASES	391
C	392
C	393
CALL CPMIX(TVAR,NN,CPMX)	394
GASCP=CPMX/AVGFW	395
H11=H	396
WI=W	397
ZLL=ZZ+0.0208333	398
PRINT 139,TC,TVAR,DTC,GASCP,DCDOV,CPV,Q,CDOV,ZZ	399
139 FORMAT(1X,'T='F9.4,' TK='F9.4,' DT='E11.4,' CP='F6.3,' DKE='E11.4,	400
1' CPP='E11.4,' Q='E11.4,' KE='E11.4,D15.7)	401
PRINT 1390,QCZI	402
QCZI=CDOV*DTC	403
GOTO113	404
C	405
C	406
C-----USE SUBROUTINE CHARPR TO GENERATE NEEDED PHYSICAL PROPERTY	407
C DATA FOR THE CHAR ZONE(HEAT CAPACITY OF THE CHAR AND THE	408

C	OVER ALL EFFECTIVE THERMAL CONDUCTIVITY OF THE GAS AND CHAR).	409
C		410
C		411
102	CALL CHARPR	412
	IF(IND.EQ.0)DTC=QCZI/CDO	413
	IND=1	414
103	IF(KEY.EQ.2)GOTO104	415
C		416
C		417
C	-----CALCULATE THE HEAT CAPACITY OF A FROZEN FLOW MIXTURE	418
C		419
C		420
	CALL CPMIX(TVAR,NN,CPMX)	421
	GASCP=CPMX/AVGEW	422
C		423
	GOTO111	424
104	IF(KOUNT.EQ.2)GOTO105	425
	CALL CHEMEQ	426
	GO TO 300	427
C		428
C	-----CHEMEQ SUBROUTINE CALCULATES THE EQUILIBRIUM COMPOSITION	429
C	OF THE REACTING GASES. IT ALSO CALCULATES THE HEAT ABSORBED	430
C	OR RELEASE DUE TO THE CHEMICAL REACTION. IN ADDITION IT	431
C	FURNISHES THE NEEDED AVERAGE MOLECULAR WEIGHT AND HEAT	432
C	CAPACITY OF THE MIXTURE.	433
C		434
105	DO110KL=2,5	435
	CALL OMEGA(TVAR,TABLE(1,1),TABLE(1,KL),KMAX,VARY)	436
C	OMEGA IS AN INTERPOLATION ROUTINE. SEE BEGINNING	437
C	OF PROGRAM FOR EXPLANATION OF VARIABLES STORED IN TABLE(I,J)	438
	II=KL-1	439
	GOTO(106,107,108,109),II	440
106	REACT=VARY	441
C	REACT=HEAT EFFECT DUE TO CHEMICAL REACTIONS. THIS	442

C	VARIABLE IS USE IN GROUP TERM BELOW. THE	443
C	UNITS OF REACT ARE(BTU/FT2-SEC-OF)	444
	GOTO110	445
107	AVGFW=VARY	446
C	AVGFW=AVERAGE MOLECULAR WEIGHT OF THE GAS MIXTURE.	447
	GOTO110	448
108	W=VARY*EPS	449
C	W=MASS FLUX(LBS/FT**2-TOTAL-SEC)	450
	GOTO110	451
109	CPMX=VARY	452
C	CPMX=HEAT CAPACITY OF THE MIXTURE(BTU/LB-MOLE-OF)	453
	GASCP=CPMX/AVGFW	454
C	GASCP=HEAT CAPACITY(BTU/LB-OF)	455
110	CONTINUE	456
	REAC1=REAC1+REACT*DELTF	457
	CPB1=CPB1+W*EPS*GASCP*DELTF	458
	CPB2=CPB2+CPS*RHO*VR*(1.-EPS)*DELTF	459
	IF(KEY.GT.1)GOTO112	460
111	ROCHAR=(WTOTAL-W)/VR	461
	CONVEG=W*GASCP	462
	CPB1=CPB1+CONVEG*DELTF	463
	CONVES=CPS*ROCHAR*VR	464
	CPB2=CPB2+CONVES*DELTF	465
	GROUP=(CONVEG+CONVES-DCDO*DTC)/CDO	466
C		467
C	DCDO=DERIVATIVE OF CDO WITH TEMPERATURE(BTU/FT-SEC-OF2)	468
C	CDO=EFFECTIVE THERMAL CONDUCTIVITY(BTU/FT-SEC-OF)	469
C	DTC=GRADIENT OF TEMPERATURE WITH DISTANCE(OF/FT)	470
C-----	THE ABOVE GROUP TERM IS FOR FROZEN CONDITION	471
C		472
	GOTO114	473
C		474
C		475
C-----	CALCULATE THE BULK DENSITY OF THE CHAR	476

C		477
C		478
112	ROCHAR=(WTOTAL-W)/VR	479
C	ROCHAR=BULK DENSITY OF THE CHAR(LBS/FT**3)	480
	CONVEG=W*GASCP	481
	CPB1=CPB1+CONVEG*DELTF	482
	CONVES=CPS*ROCHAR*VR	483
	CPB2=CPB2+CONVES*DELTF	484
	REAC1=REAC1+REACT*DELTF	485
	GROUP=(CONVEG+CONVES+REACT-DCDO*DTC)/CDO	486
C		487
C	VR=SURFACE RECESSION VELOCITY(FT/SEC)	488
C	THE ABOVE GROUP TERM HOLDS FOR EQUILIBRIUM IN THE CHAR	489
	GOTO114	490
113	GROUP=(W*GASCP+CPV*RHO*VR+Q/DTC-DCDOV*DTC)/CDOV	491
C		492
C	-----THE ABOVE GROUP TERM IS USED DURING THE DEPOLYMERIZATION OF	493
C	THE VIRGIN PLASTIC COMPOSITE.	494
C		495
114	A=DTC	496
	DELG1=H*G(A)	497
	DELF1=H*F(A)	498
	DELG2=H*G(A+DELF1/2.)	499
	DELF2=H*F(A+DELF1/2.)	500
	DELG3=H*G(A+DELF2/2.)	501
	DELF3=H*F(A+DELF2/2.)	502
	DELG4=H*G(A+DELF3)	503
	DELF4=H*F(A+DELF3)	504
	DTC=DTC+(DELF1+2.*(DELF2+DELF3)+DELF4)/6.	505
	IF(IND.EQ.0)GOTO115	506
	QCZ=CDO*DTC	507
115	TPREV=TC	508
	IF(H.LT.0.8F-8)GOTO117	509
	TC=TC+(DELG1+2.*(DELG2+DELG3)+DELG4)/6.	510

	GOTO118	511
117	IF(K10.EQ.0)TTTT=TC	512
	K10=1	513
	DTCC=DTC	514
	TTTT=TTTT+H11*DTCC	515
	TC=TTTT	516
118	DELTF=TC-TPREV	517
	DELTK=DELTF/1.8	518
C		519
C-----	COMPARE THE TEMPERATURE CALCULATED WITH THE MAXIMUM VALUE.	520
C		521
C		522
138	ZPREV=ZZ	523
	ZZ=ZZ+H11	524
	IF(TC.GT.1000.)H=2.E-5	525
	IF(KEY.EQ.1)GOTO141	526
	IF(TC.GT.1500.)H=2.E-6	527
	IF(TC.GT.3000.)H=1.E-6	528
	IF(TC.GT.3500.)H=0.5E-6	529
	H11=H	530
	Z=ZZ	531
141	IF(TC.GT.TFMAX)GOTO150	532
	N=N+1	533
	IF(TVAR.LE.TCHAR)ZZ=ZZ	534
	IF(TVAR.LE.TCHAR)GOTO101	535
	IF(ZZ.GT.ZZ)GOTO101	536
140	PRINT 142,TC,H,DTC,GASCP,DCDO,GROUP,REACT,CDO	537
142	FORMAT(1X,'TF='F9.4,' H='E14.6,' DT='E11.5,' CP='F6.4,' DKE='E11	538
	1.5,' GRP='E12.5,' Q='E11.4,' KE='E11.5)	539
	PRINT 1140,AVGFW,W,CPMX,TVAR,KMAX,CPS,GASCP,RHO,QCZ	540
1140	FORMAT(1X,'AVGFW='F 7.3,' W='F 7.5,' CPMX='E9.2,' TVAR='F7.2,	541
	1' KMAX='I5,' CPS='F 6.3,' GASCP='F 6.4,' RHO='F8.4,' QCZ='F10.2)	542
	IF(TC.GT.2600.)ZINC=1.2E-5	543
	ZZ=ZZ+ZINC	544

Z1(K1)=ZPREV	545
T1(K1)=TPREV	546
CHARDN(K1)=ROCHAR	547
TOK(K1)=TVAR	548
C	549
C	550
C-----STORE THE TEMPERATURE PROFILE FOR LATER USE IN THE SOLUTION	551
C      OF THE MOMENTUM EQUATION.	552
C	553
C	554
PRINT 153,REAC1,CPB1,CPB2,ZPREV,K1	555
153  FORMAT(1X,'REAC1='E15.7,' CPB1='E15.7,' CPB2='E15.7,	556
1' ZPREV='E15.7,I5/)	557
K1=K1+1	558
IF(K1.GT.199)K1=199	559
GOTO101	560
150  TL=TC	561
C      TL=FINAL TEMPERATURE	562
PRINT 1140,AVGFW,W,CPMX,TVAR,KMAX,CPS,GASCP,RHO,QCZ	563
PRINT 142,TC,H,DTC,GASCP,DCDO,GROUP,REACT,CDO	564
PRINT 153,REAC1,CPB1,CPB2,ZPREV,K1	565
T1(K1)=TL	566
C      THE TEMPERATURE PROFILE HAS BEEN DEFINED	567
DELTT=TL-T1(1)	568
C      DELTT=TEMPERATURE DROP ACROSS THE CHAR(OF)	569
Z1(K1)=ZZ	570
CHARDN(K1)=ROCHAR	571
TOK(K1)=(TC+459.69)/1.8	572
PRINT 154	573
154  FORMAT(1H1, 7X,'T(OF)', 9X,'T(OK)', 11X,'Z')	574
DO 156 I=1,K1	575
PRINT 155,T1(I),TOK(I),Z1(I)	576
155  FORMAT(1X,4E15.7)	577
156  CONTINUE	578

	DISTAN=Z1(K1)-Z1(1)	579
C	DISTAN IS THE THICKNESS OF THE CHAR.	580
C		581
C	-----CALCULATION OF THE PRESSURE PROFILE IN THE	582
C	CHAR USING SIMPSON'S RULE FOR THE INTEGRATION	583
C	OF THE MOMENTUM EQUATION FOLLOWS.	584
C		585
	JS=39	586
C	JS=NUMBER OF SLICES IN THE CHAR	587
	HS=DISTAN/FLOAT(JS)	588
C	HS=INCREMENT OF GRID(IN FEET)	589
C	-----INITIALIZE	590
	SIMP1=0.	591
	SIMP2=0.	592
	ITEMP=K1	593
C	ITEMP=TOTAL NUMBER OF TEMPERATURE POINTS STORED	594
	LS=JS+1	595
	WFLUX(1)=WI	596
	ZX(LS)=Z1(K1)	597
	TP(LS)=TL	598
	P(LS)=PL	599
C		600
C	-----THE INTEGRATION OF THE MOMENTUM EQUATION IS PERFORMED	601
C	FROM THE FRONT SURFACE OF THE CHAR TO THE BACK SURFACE	602
C	THE INTEGRATION OF THE ENERGY EQUATION, ON THE OTHER	603
C	HAND, WAS PERFORMED FROM THE VIRGIN MATERIAL TO THE FRONT	604
C	SURFACE OF THE CHAR. BECAUSE THE DIRECTION OF INTEGRATION	605
C	OF BOTH EQUATIONS ARE DIFFERENT IT IS NECESSARY TO RE-	606
C	DEFINE Z=0. AT THE FRONT SURFACE OF THE CHAR.	607
C		608
	ACON1=2.6693E-3	609
	ACON5=2.42/3600.	610
	ACON7=778.16/32.2	611
	MS=20	612

HSIMPI=HS/FLOAT(MS)	613
MP=MS+1	614
DO260N=1,JS	615
NBAR=N-1	616
HN=NBAR	617
LO=LS-NBAR	618
ZX(LO)=ZX(LS)-HN*HS	619
ZY(MP)=ZX(LO)	620
C DEFINE MP AS THE TOTAL NO. OF POINT OVER WHICH SIMPSON'S	621
C RULE IS TO BE APPLIED	622
DO241M=1,MP	623
MBAR=M-1	624
HM=MBAR	625
MO=MP-MBAR	626
ZY(MO)=ZY(MP)-HM*HSIMPI	627
ZVAR=ZY(MO)	628
IF(ZVAR.LT.Z1(1))ZVAR=Z1(1)	629
C	630
C-----FOR A SPECIFIED CHAR DISTANCE OBTAIN THE	631
C CORRESPONDING TEMPERATURE FROM THE TEMPE-	632
C RATURE PROFILE	633
C	634
CALL OMEGA(ZVAR,Z1,T1,ITEMP,TVIS)	635
C TVIS IS THE INTERPOLATED TEMPERATURE IN OF	636
C WHICH CORRESPONDS TO THE VALUE OF ZVAR	637
TK=(459.69+TVIS)/1.8	638
C TK=TEMPERATURE IN KELVIN	639
DO205I=1,NC	640
TKE=TK/EK(I)	641
C	642
C	643
C-----FOR THE VALUE OF INTERPOLATED TEMPERATURE FIND	644
C THE CORRESPONDING COLLISION INTEGRAL TO CALCULATE	645
C THE PURE GAS VISCOCITY USING THE METHOD OF WILKE-JOHNSON	646



C	CALL OMEGA(TKE,XTKE,ZOMGA,NDATA,OMGA)	647
		648
C		649
C	OMGA=COLLISION INTEGRAL	650
C		651
205	VIS(1)=2.6693E-3*SQRT(FW(1)*TK)/(SIG(1)**2*OMGA)	652
	IF(NC.EQ.1)GOTO237	653
	IF(KEY.GT.1)GOTO206	654
	VMIX=0.	655
	WFLUX(LO)=WI	656
	GO TO 222	657
206	TVAR=TK	658
	DO218KL=3,NN5	659
		660
C		661
C	THE FIFTH VARIABLE STORED IN TABLE IS CPMX. THIS	662
C	VARIABLE IS NOT USED IN THE SOLUTION OF THE MOMENTUM	663
C	EQUATION. SO ITS INTERPOLATION IS BYPASSED.	664
C		665
	IF(KL.EQ.5)GOTO218	666
C		667
C	INTERPOLATE FOR THE DATA GENERATED IN CHEMEQ	668
C		669
	CALL OMEGA(TVAR,TABLE(1,1),TABLE(1,KL),KMAX,VARY1)	670
	IF(KL.GT.5)GOTO216	671
C		672
C	KMAX=NUMBER OF DATA POINTS STORED	673
C		674
	IF(KL.EQ.4)GOTO215	675
	AVGFW=VARY1	676
	GOTO218	677
215	W=VARY1	678
	GOTO217	679
216	Y(KL-5)=VARY1	680
	IF(VARY1.GT.0.)GOTO217	

	Y(KL-5)=1.E-10	681
217	IF(M.GT.1)GOTO218	682
	TP(LO)=TVIS	683
	WFLUX(LO)=W	684
	KYCOMP=KL-5	685
	YCOMP(KYCOMP,LO)=Y(KYCOMP)	686
218	CONTINUE	687
	VMIX=0.	688
	GOTO224	689
222	IF(M.GT.1)GOTO224	690
	DO 223 I=1,NS	691
	YCOMP(I,LO)=XMOL(I)	692
	WFLUX(LO)=W	693
223	TP(LO)=TVIS	694
224	DO 236 J=1,NC	695
	TERM=1.	696
	DO230L=1,NC	697
	IF(L.EQ.J)GOTO230	698
	TOPV=(1.+SQRT(VIS(J)/VIS(L))*SQRT(SQRT(FW(L)/FW(J))))**2	699
	BOTV= SQRT(2.)*SQRT(1.+FW(J)/FW(L))*2.	700
	PHIV=TOPV/BOTV	701
	TERM=TERM+PHIV*(Y(L)/Y(J))	702
230	CONTINUE	703
	VMIX=VMIX+VIS(J)/TERM	704
236	CONTINUE	705
	GOTO238.	706
237	VISCOS=VIS(I)*ACON5	707
C	ACON5=2.42/3600.	708
	GOTO239	709
238	VISCOS=VMIX*ACON5	710
239	PROD(MO)=TVIS*VISCOS*W/AVGFW	711
	TT(MO)=TVIS/AVGFW*(W**2)	712
241	CONTINUE	713
	ZX(LO-1)=ZX(LO)-HS	714

C	INTEGRATE USING SIMPSONS RULF	715
	SUM1=0.	716
	SUM2=0.	717
	SUM3=0.	718
	SUM4=0.	719
	M0DD=MP-2	720
	DO255KP=3,M0DD,2	721
	SUM1=SUM1+2.*PROD(KP)	722
255	SUM3=SUM3+2.*TT(KP)	723
	MEVEN=MP-1	724
	DO256KP=2,MEVEN,2	725
	SUM2=SUM2+4.*PROD(KP)	726
256	SUM4=SUM4+4.*TT(KP)	727
	SIMP1=(HSIMP1/3.0)*(PROD(1)+SUM1+SUM2+PROD(MP))+SIMP1	728
	SIMP2=(HSIMP1/3.0)*(TT(1)+SUM3+SUM4+TT(MP))+SIMP2	729
C	FR2=778.16/32.2	730
	P(LO-1)=SQRT(PL**2+(2.*RR)*FR2*(ALPHA*SIMP1+BETA*SIMP2))	731
260	CONTINUE	732
C		733
C		734
C	-----CALCULATE THE SURFACE HEAT FLUX,QL,THE RERADIATION,QR,	735
C	AND THE TOTAL AERODYNAMIC HEATING,QA.	736
C		737
C		738
	IF(KEY.GT.1)GOTO261	739
	QL=QCZ	740
	GOTO262	741
261	QL=QCZ	742
262	QR=EMIS*SIGMA*(TL+459.69)**4	743
	QA=QL+QR	744
C		745
	TP(1)=T1(1)	746
C	PRINT INPUT PARAMETERS	747
C		748

2603 PRINT 597	749
597 FORMAT(1H1/////////)	750
IF(KEY.EQ.2)GOTO5982	751
PRINT 5981	752
5981 FORMAT(35X,'INDEPTH FLOW ANALYSIS(FROZEN FLOW)')//)	753
5982 PRINT 5984	754
5984 FORMAT(35X,'INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)')//)	755
5986 PRINT 5990	756
5990 FORMAT(12X,51H	757
THEORETICAL/	758
1/)	759
PRINT600,T1(1),NC	760
600 FORMAT(18X,'CHAR BACK TEMPERATURE (OF)='F7.1,13X,'NUMBER OF GAS CO	761
MPONENTS='I3/)	762
PRINT 601,DTCII,RHOII	763
601 FORMAT(18X,'INITIAL SLOPE(OF/FT)='F8.1,12X,'INITIAL DENSITY OF COM	764
1POSITE(LBS/FT**3)='F6.2/)	765
THICK=DISTAN*12.	766
THICK1=Z1(1)*12.	767
PRINT 602,THICK,THICK1	768
602 FORMAT(18X,'THICKNESS OF CHAR(INCHES)='F8.6,6X,'THICKNESS OF DECOM	769
1POSITION ZONE='F8.6/)	770
QCZZ=QCZ-QCZI	771
PRINT 604,WTOTAL,WFLUX(LS)	772
604 FORMAT(18X,'TOTAL MASS FLUX(LBS/FT2-SEC)='F7.6,6X,29HGAS MASS FLUX	773
1 AT THE SURFACE=,1X,F7.6/)	774
PRINT 611,TFMAX,VR	775
611 FORMAT(18X,'FRONT SURFACE TEMPERATURE(OF)='F6.1,5X,'SURFACE RECESS	776
1ION VELOCITY(FT/SEC)='F7.5/)	777
PRINT 603,QCZZ,QCZI	778
603 FORMAT(25X,'RATE OF HEAT ABSORBED IN THE CHAR ZONE(BTU/FT**2-SEC)=	779
1'F9.3,7/25X,'RATE OF HEAT ABSORBED IN THE DECOMPOSITION ZONE(BTU/F	780
1T2-SEC)='F9.3/)	781
HCHAR=QCZZ/QCZ*100.	782
HDECOM=QCZI/QCZ*100.	

SUM=REAC1*CPB1+CPB2	783
HGAS=CPB1/SUM*100.	784
HSOLID=CPB2/SUM*100.	785
HREACT=REAC1/SUM*100.	786
PRINT 605,HCHAR	787
605 FORMAT(25X,'PERCENT OF TOTAL HEAT ABSORBED IN THE CHAR ZONE='E15.7	788
1/)	789
PRINT 606,HDECOM	790
606 FORMAT(25X,'PERCENT OF TOTAL HEAT ABSORBED IN DECOMP-ZONE='E15.7/)	791
PRINT 607,HGAS	792
607 FORMAT(25X,'PERCENT OF HEAT ABSORBED BY THE GAS IN THE CHAR ZONE='	793
1E15.7/)	794
PRINT 608,HSOLID	795
608 FORMAT(25X,'PERCENT OF HEAT ABSORBED BY THE SOLIDS IN THE CHAR ZON	796
1E='E15.7/)	797
PRINT 610,HREACT	798
610 FORMAT(25X,'PERCENT OF HEAT ABSORBED BY REACTION IN THE CHAR ZONE=	799
1'E15.7/)	800
PRINT586	801
586 FORMAT(1H1)	802
C	803
C-----PRINT OUTPUT PARAMETERS CORRESPONDING TO JS, GRID SIZE	804
C	805
IKE=1	806
MIKE=5	807
LIKE=1	808
2602 PRINT 597	809
2662 PRINT 5984	810
IF(LIKE.GT.1)GO TO 265	811
PRINT2650,DELTT	812
2650 FORMAT(35X,23HTEMPERATURE DROP (OF) =,1X,F20.1/)	813
DELP=(P(1)-PL)	814
PRINT2651,DELP	815
2651 FORMAT(35X,24HPRESSURE DROP (LB/FT2) =,1X,F19.1/)	816

PRINT2652,QL	817
2652 FORMAT(35X,33HSURFACE HEAT FLUX (BTU/FT2-SEC) =,1X,F10.2/)	818
PRINT2653,QR	819
2653 FORMAT(35X,32HRADIANT HEAT FLUX BTU/FT2-SEC)=,1X,F11.2/)	820
PRINT2654,QA	821
2654 FORMAT(35X,35HAERODYNAMIC HEAT FLUX(BTU/FT2-SEC)=,1X,F8.2//)	822
265 PRINT2720,(ZX(KK),KK=IKE,MIKE)	823
2720 FORMAT(14X,15HCHAR DEPTH (FT),6X,5F13.4)	824
PRINT2721,(TP(KK),KK=IKE,MIKE)	825
2721 FORMAT(14X,16HTEMPERATURE (OF),5X,5F13.1)	826
PRINT2730,(P(KK),KK=IKE,MIKE)	827
2730 FORMAT(14X,17HPRESSURE (LB/FT2),4X,5F13.1)	828
PRINT2723,(WFLUX(KK),KK=IKE,MIKE)	829
2723 FORMAT(14X,21HMASS FLUX(LB/FT2-SEC),5F13.4/)	830
PRINT2724	831
2724 FORMAT(14X,66H GAS COMPONENT COMPOSITION (	832
1MOLE/MOLE GAS)/)	833
IF(KEY.GT.1)GOTO2727	834
DO 2728 KICK=1,LS	835
DO2728LL=1,NS	836
YCOMP(LL,KICK)=YI(LL)	837
2728 CONTINUE	838
2727 DO2729LL=1,NS	839
YCOMP(LL,1)=YI(LL)	840
PRINT 2725,LL,SPCIE1(LL),SPCIE2(LL),(YCOMP(LL,KK),KK=IKE,MIKE)	841
2725 FORMAT(12X,I2,2X,2A3,11X,5E13.4)	842
2729 CONTINUE	843
IF(MIKE.GE.LS)GO TO 2800	844
LIKE=LIKE+1	845
MIKE=MIKE+5	846
IKE=IKE+5	847
GO TO 2602	848
2800 PRINT586	849
300 STOP	850

END

851

	SUBROUTINE INDPH(TC,CDOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,	INDP	1
	1 DELTKK,N,DELZ,VR,W,H)	INDP	2
C		INDP	3
C		INDP	4
C		INDP	5
	DIMENSION DRHODT(5)	INDP	6
C		INDP	7
C-----	INDPTH SUBROUTINE CALCULATES THE PHYSICAL PROPER-	INDP	8
C	TIES FOR THE VIRGIN MATERIAL AND PYROLYSIS GASES.	INDP	9
C		INDP	10
C	T=TEMPERATURE IN FARENHEIT.	INDP	11
	IF(N.GT.1)GOTO2	INDP	12
	DCDOV=.338983E-8	INDP	13
	READ 1,A,B,C,D,E	INDP	14
C	A THROUGH E ARE CONSTANT FOR THE HEAT CAPACITY OF THE	INDP	15
C	VIRGIN MATERIAL.	INDP	16
	1 FORMAT(5E12.6)	INDP	17
C	CDOV=THERMAL CONDUCTIVITY OF THE VIRGIN MATERIAL	INDP	18
C	(BTU/(FT-SEC-OF))	INDP	19
	2 CDOV=1.266102E-5+.338983E-8*TC	INDP	20
	PRINT 10,H,DELZ	INDP	21
10	FORMAT(1X,'IN INDPH H='E15.7,' DELZ='E15.7)	INDP	22
C	DCDOV=RATE OF CHANGE OF CDOV WITH THEMPERATURE.	INDP	23
	T=TC	INDP	24
	IF(T.GT.750.)GOTO3	INDP	25
	T2=TC*T	INDP	26
	T3=TC*T2	INDP	27
	T4=TC*T3	INDP	28
C		INDP	29
C	CPV=HEAT CAPACITY OF THE VIRGIN MATERIAL(BTU/LB-OF)	INDP	30
	CPV=A+B*T+C*T2+D*T3+E*T4	INDP	31
	3 GASCP=.62	INDP	32
C		INDP	33
	CALL PHMCR(TVAR,DELTKK,QPHNLC,QMICRO,N)	INDP	34



C	IF(TVAR.GE.789.)GOTO200	INDP	35
		INDP	36
C	CALL NYLON(TVAR,DELTKK,QNYLON)	INDP	37
	GOTO210	INDP	38
	200 QNYLON=0.	INDP	39
		INDP	40
C	210 CALL DENSITY(RHO,TVAR,DELZ,VR,N,DRHODT,W,H)	INDP	41
	Q=(QNYLON*DRHODT(1)+QPHNLC*DRHODT(2)+QMICRO*DRHODT(3))*(-1.8)	INDP	42
	RETURN	INDP	43
	END	INDP	44
		INDP	45

C	SUBROUTINE PHMCR(T,DELT,OPHNLC,QMICRO,K6)	PHMC	1
C		PHMC	2
C		PHMC	3
C	DIMENSION A(4),B(4),C(4),D(4),E(4),A1(4),B1(4),C1(4),D1(4),E1(4)	PHMC	4
C		PHMC	5
C		PHMC	6
C	-----THIS SUBROUTINE COMPUTES THE HEAT OF PYROLYSIS OF PHENOLIC,	PHMC	7
C		PHMC	8
C		PHMC	9
C	BASED ON THE DATA OF SYKES AND NELSON(THERMOANALYSIS OF	PHMC	10
C	ABLATION MATERIALS)	PHMC	11
	IF(K6.GT.1)GOTO4	PHMC	12
	NUMBER=4	PHMC	13
	AREA=1350.	PHMC	14
	AREA1=1464.	PHMC	15
C	READ1,NUMBER,AREA,AREA1	PHMC	16
	1 FORMAT(I6,2E10.8)	PHMC	17
	DO2I=1,NUMBER	PHMC	18
	READ3,A(I),B(I),C(I),D(I),E(I)	PHMC	19
	2 READ3,A1(I),B1(I),C1(I),D1(I),E1(I)	PHMC	20
	3 FORMAT(5E12.8)	PHMC	21
	4 IF(T.LT.623.)GOTO5	PHMC	22
	IF(T.GT.1073.)GOTO5	PHMC	23
	I=1	PHMC	24
	IF(T.GT.748..AND.T.LT.798.)I=2	PHMC	25
	IF(T.GT.798..AND.T.LT.898.)I=3	PHMC	26
	IF(T.GT.898.)I=4	PHMC	27
	DT=(T-623.)	PHMC	28
	DT2=DT*DT	PHMC	29
	DT3=DT2*DT	PHMC	30
	DT4=DT3*DT	PHMC	31
C	CALCULATE THE HEAT OF PYROLYSIS OF PHENOLIC(OPHNLC)	PHMC	32
	H=A(I)+B(I)*DT+C(I)*DT2+D(I)*DT3+E(I)*DT4	PHMC	33
	OPHNLC=H*DELT*69.312/AREA	PHMC	34

C		PHMC	35
C	69.312=TOTAL HEAT ABSORBED BY THE DECOMPOSITION OF	PHMC	36
C	PHENOLIC IN CAL/GRAM.	PHMC	37
C		PHMC	38
C	CALCULATE THE HEAT OF PYROLYSIS OF PHENOLIC MICRO-	PHMC	39
C	BALLOONS(QMICRO)	PHMC	40
	I=1	PHMC	41
	IF(T.GT.713..AND.T.LT.798.)I=2	PHMC	42
	IF(T.GT.798..AND.T.LT.913.)I=3	PHMC	43
	IF(T.GT.913.)I=4	PHMC	44
	H=A1(I)+B1(I)*DT+C1(I)*DT2+D1(I)*DT3+E1(I)*DT4	PHMC	45
	QMICRO=H*DELT*90.822/AREA1	PHMC	46
C	90.822=TOTAL HEAT ABSORBED BY THE DECOMPOSITION OF	PHMC	47
C	PHENOLIC MICRO-BALLOONS IN CAL/GRAM.	PHMC	48
	RETURN	PHMC	49
5	QPHNLC=0.	PHMC	50
	QMICRO=0.	PHMC	51
6	RETURN	PHMC	52
	END	PHMC	53

SUBROUTINE NYLON(T,DELT,QNYLON)	NYLO	1
C	NYLO	2
C	NYLO	3
C-----THIS SUBROUTINE COMPUTES THE HEAT OF PYROLYSIS OF NYLON	NYLO	4
C BASED ON THE DATA OF SYKES AND NELSON(THERMOANALYSIS OF	NYLO	5
C ABLATION MATERIALS)	NYLO	6
C	NYLO	7
C SLOPF=SLOPE OF LINE OBTAIN FROM SYKES AND NELSON'S DATA.	NYLO	8
QNYLON=0.	NYLO	9
SLOPE=0.6086957	NYLO	10
C	NYLO	11
AREA=1122.	NYLO	12
C AREA=AREA UNDER CURVE OF FIGURE-2(DIFFERENTIAL THERMAL	NYLO	13
C ANALYSIS) BY SYKES AND NELSON	NYLO	14
CONST=150.5738/AREA	NYLO	15
IF(T.LT.647.)GOTO4	NYLO	16
IF(T.GT.699.)GOTO2	NYLO	17
IF(T.GE.689..AND.T.LE.699.)GOTO1	NYLO	18
H=SLOPE*(T-647.)	NYLO	19
GOTO3	NYLO	20
1 H=24.4	NYLO	21
GOTO3	NYLO	22
2 DH=SLOPE*(T-693.)	NYLO	23
H=28.0-DH	NYLO	24
IF(T.GE.739.)H=0.	NYLO	25
3 QNYLON=DELT*H*CONST	NYLO	26
4 RETURN	NYLO	27
END	NYLO	28

C	SUBROUTINE OMEGA (VAR,X,F,IMAX,SOM)	OMEG	1
C		OMEG	2
C		OMEG	3
C		OMEG	4
C	-----THIS PROGRAM PERFORMS LAGRANGIAN INTERPOLATION	OMEG	5
C	WITH NON-EQUAL STEP SIZE BETWEEN POINTS	OMEG	6
C	F=DEPENDANT VARIABLE	OMEG	7
C	X=INDEPENDENT VARIABLE	OMEG	8
C	VAR=VALUE OF X FOR WHICH CORRESPONDING VALUE OF	OMEG	9
C	F IS DESIRED BY INTERPOLATION	OMEG	10
C	IMAX=NUMBER OF POINTS IN ARRAY X OR F	OMEG	11
C	SOM=VALUE OF INTERPOLATED DEPENDENT VARIABLE	OMEG	12
C	NPTS=NUMBER OF POINTS USED FOR INTERPOLATION	OMEG	13
C		OMEG	14
	DIMENSION X( 1),F( 1),XN(350),FN(350)	OMEG	15
	COMMON/KK/IP	OMEG	16
	NPTS=3	OMEG	17
607	XUP=1.E30	OMEG	18
	DO6111=1,IMAX	OMEG	19
	T=VAR-X(I)	OMEG	20
	IF(T.GE.0.)GOTO609	OMEG	21
608	T=-T	OMEG	22
609	IF(T.GE.XUP)GOTO611	OMEG	23
610	IP=I	OMEG	24
	XUP=T	OMEG	25
611	CONTINUE	OMEG	26
	IN=1	OMEG	27
	NPP=NPTS+1	OMEG	28
	DO6181=1,NPP	OMEG	29
	FN(I)=F(IP)	OMEG	30
	XN(I)=X(IP)	OMEG	31
	IF(IN.GT.0)GOTO613	OMEG	32
612	IQ=IP-I	OMEG	33
	GOTO615	OMEG	34

613	IQ=IP+I	OMEG	35
	IF( IMAX.GE.IQ)GOTO615	OMEG	36
614	IP=IP-1	OMEG	37
	GOTO618	OMEG	38
615	IF( IQ.GT.0)GOTO617	OMEG	39
616	IP=IP+1	OMEG	40
	GOTO618	OMEG	41
617	IP=IQ	OMEG	42
	IN=-IN	OMEG	43
618	CONTINUE	OMEG	44
	SOM=0.	OMEG	45
	FACT=1.	OMEG	46
	DO620J=1,NPTS	OMEG	47
	SOM=SOM+FACT*FN(I)	OMEG	48
	DO619I=J,NPTS	OMEG	49
	IQ=I-J+1	OMEG	50
619	FN(IQ)=(FN(IQ+1)-FN(IQ))/(XN(I+1)-XN(IQ))	OMEG	51
620	FACT=FACT*(VAR-XN(J))	OMEG	52
	RETURN	OMEG	53
	END	OMEG	54

	SUBROUTINE THERM1	THER	1
C	THIS SUBPROGRAM CALCULATES THE HEAT OF FORMATION AND	THER	2
C	THE ENTROPY OF EACH CHEMICAL SPECIE	THER	3
	COMMON/KA/S1(6),S2(6),S3(6),S4(6),S5(6),S6(6),A11(6),	THER	4
	1A22(6),A33(6),A44(6),A55(6),A66(6),AA(30,6),JCODE(6)	THER	5
	COMMON/KB/AT(30),BI(30),CI(30),DI(30),EI(30),FI(30),GI(30),	THER	6
	2AII(30),BII(30),CII(30),DII(30),EII(30),FII(30),GII(30),	THER	7
	3TLOW(30)	THER	8
	COMMON/KC/ICODE(30),Y(30),XMW(30)	THER	9
	COMMON/KEE/PL,RR,TZERO,EPS,KEY,NN,NQ,MM	THER	10
	COMMON/KG/ENT(30),S(30),ENT1(30),T	THER	11
C	S1....S6=EMPIRICAL CONSTANTS FOR THE HIGH TEMPERATURE	THER	12
C	ENTHALPY FIT OF THE CONSTITUENT ELEMENTS	THER	13
C	A11..A66=EMPIRICAL CONSTANTS FOR THE LOW TEMPERATURE	THER	14
C	ENTHALPY FIT OF THE CONSTITUENT ELEMENTS	THER	15
C	AT....GI=EMPIRICAL CONSTANTS FOR THE HIGH TEMPERATURE	THER	16
C	FIT OF THE CHEMICAL SPECIES	THER	17
C	AII..BII=EMPIRICAL CONSTANTS FOR THE LOW TEMPERATURE	THER	18
C	FIT OF THE CHEMICAL SPECIES	THER	19
	DIMENSION CPDT1(6)	THER	20
C	ENT(I)=HEAT OF FORMATION AT ANY TEMPERATURE T	THER	21
C	ENT1(I)=SENSIBLE ENTHALPY GAIN+CHEMICAL ENERGY(HEAT	THER	22
C	OF FORMATION AT 298.16 OK)	THER	23
C	CPDT1(J)=SENSIBLE ENTHALPY GAIN OF THE ELEMENTS	THER	24
C	TLOW(I)=TEMPERATURE AT WHICH ONE MUST CHANGE FROM ONE FIT	THER	25
C	TO THE OTHER OR, THE MIN TEMP OF HIGH TEMP FIT.	THER	26
C	S=ENTROPY	THER	27
C	NN=NUMBER OF GAS SPECIES	THER	28
C	NQ=NUMBER OF GAS+SOLID SPECIES	THER	29
C	MM=NUMBER OF CONSTITUENT ELEMENTS	THER	30
C	T=TEMPERATURE IN OK.	THER	31
	T1=T	THER	32
	T2=T1*T	THER	33
	T3=T2*T	THER	34

	T4=T3*T	THER	35
	T5=T4*T	THER	36
	A1=T1	THER	37
	A2=T2/2.	THER	38
	A3=T3/3.	THER	39
	A4=T4/4.	THER	40
	A5=T5/5.	THER	41
C	CALCULATE THE HEAT OF FORMATION, ENT, AND THE ENTROPY S.	THER	42
	DO 8 I=1, NQ	THER	43
	IF (T.LT.TLOW(I)) GOTO3	THER	44
	ENT1(I)=(A1(I)*A1+B1(I)*A2+C1(I)*A3+D1(I)*A4+E1(I)*A5	THER	45
	1+F1(I))*RR	THER	46
	S(I)=(A1(I)*ALOG(T)+B1(I)*A1+C1(I)*A2+D1(I)*A3+E1(I)*A4+G1(I))*RR	THER	47
	IF (I.GT.1) GOTO5	THER	48
	DO2 J=1, MM	THER	49
2	CPDT1(J)=(S1(J)*A1+S2(J)*A2+S3(J)*A3+S4(J)*A4+S5(J)*A5+S6(J))*RR	THER	50
	GOTO5	THER	51
3	ENT1(I)=(A11(I)*A1+B11(I)*A2+C11(I)*A3+D11(I)*A4+E11(I)*A5	THER	52
	1+F11(I))*RR	THER	53
	S(I)=(A11(I)*ALOG(T)+B11(I)*A1+C11(I)*A2+D11(I)*A3+E11(I)*A4	THER	54
	1+G11(I))*RR	THER	55
	IF (I.GT.1) GOTO5	THER	56
	DO4 J=1, MM	THER	57
4	CPDT1(J)=(A11(J)*A1+A22(J)*A2+A33(J)*A3+A44(J)*A4+A55(J)*A5	THER	58
	1+A66(J))*RR	THER	59
5	RSUM=0.	THER	60
C	RSUM IS THE SENSIBLE ENTHALPY OF THE CONSTITUENT ELEMENTS	THER	61
C	OF THE ITH SPECIE (AT TEMPERATURE T(OK) WITH RESPECT TO THE	THER	62
C	STANDARD STATE P=1 ATM AND T=298.16 OK).	THER	63
	DO7 J=1, MM	THER	64
	IF (JCODE(J).EQ.1) GOTO6	THER	65
C	WHEN JCODE(J)=0, THE CONSTITUENT ELEMENT HAS BEEN ASSUMED TO BE	THER	66
C	IN ITS BI-MOLECULAR FORM. FOR EXAMPLE HYDROGEN IS TAKEN TO BE	THER	67
C	H2. WHEN JCODE(J)=1, THE CONSTITUENT ELEMENT HAS BEEN ASSUMED TO	THER	68



C	BE ITS UNI-MOLECULAR,OR ATOMIC FORM. FOR EXAMPLE CARBON IS TAKEN	THER	69
C	TO BE C.	THER	70
C	AA(I,J) IS THE FORMULA NUMBER. IT GIVES THE GRAM-ATOMS OF	THER	71
C	ELEMENT J IN SPECIE I. EXAMPLE,CH4(METHANE),AA(I,J) FOR	THER	72
C	CARBON IS 1. FOR HYDROGEN IS 4.	THER	73
	RSUM=RSUM+0.500*AA(I,J)*CPDT1(J)	THER	74
	GOTO7	THER	75
6	RSUM=RSUM+AA(I,J)*CPDT1(J)	THER	76
7	CONTINUE	THER	77
	ENT(I)=ENT1(I)-RSUM	THER	78
	IF(ABS(ENT(I)).LT.3.)ENT(I)=0.	THER	79
8	CONTINUE	THER	80
	RETURN	THER	81
	END	THER	82

SUBROUTINE DENSITY(RHO,T,DELZ,VR,K6,DRHODT,W,H)	DN SI	1
C	DN SI	2
C	DN SI	3
C-----THIS SUBROUTINE CALCULATES THE DENSITY OF PHENOLIC-NYLON	DN SI	4
C COMPOSITES AS A FUNCTION OF TEMPERATURE--BASED ON DATA	DN SI	5
C OF SYKES AND NELSON(THERMOANALYSIS OF ABLATION MATERIALS)	DN SI	6
C	DN SI	7
C	DN SI	8
COMMON/KL/WTOTAL,RHOI	DN SI	9
DIMENSION RHOI(5),RHOT(5),RHOC(5),A(7),E(7),RATER(7),	DN SI	10
1DRHODT(5),XN(5,7),FRAC(5),RHOVOL(5)	DN SI	11
DIMENSION MASFRC(5),MASFLX(5),VOLUME(5),VOLFRC(5),DELFLX(5)	DN SI	12
DIMENSION RHOCC(5),DRHO(5)	DN SI	13
INTEGER COMPST	DN SI	14
REAL MASFRC,MASFLX	DN SI	15
IF(K6.GT.1)GOTO7	DN SI	16
C	DN SI	17
C	DN SI	18
C-----READ INPUT	DN SI	19
C	DN SI	20
C	DN SI	21
READ 1,COMPST,NREACT	DN SI	22
1 FORMAT(2I6)	DN SI	23
C	DN SI	24
C COMPST=NUMBER OF COMPOSITE MATERIALS DEGRADING DURING	DN SI	25
C ABLATION.	DN SI	26
C NREACT=NUMBER OF PSEUDO-KINETIC REACTIONS USED TO DES-	DN SI	27
C CRIBE THE DEGRADATION OF THE ABLATIVE COMPOSITES.	DN SI	28
C	DN SI	29
C	DN SI	30
C	DN SI	31
C-----INITIALIZATION OF XN(I,J),WHICH IS THE ORDER OF THE	DN SI	32
C REACTION	DN SI	33
C	DN SI	34

C		DNSI	35
	DO2J=1,NREACT	DNSI	36
	DO2I=1,COMPST	DNSI	37
	2 XN(I,J)=0.	DNSI	38
C		DNSI	39
C	A(J)=FREQUENCY FACTOR(SEC-1)	DNSI	40
C	E(J)=ENERGY OF ACTIVATION(JOULE/(MOLE))	DNSI	41
C		DNSI	42
C		DNSI	43
	R=8.314	DNSI	44
C	R=8.314(JOULES/(MOLE-OK))	DNSI	45
C		DNSI	46
C		DNSI	47
C	RHOI(1)=68.6(NYLON)	DNSI	48
C	RHOI(2)=80.0(PHENOLIC RESIN)	DNSI	49
C	RHOI(3)=17.8(PHENOLIC-MICROBALLOONS)	DNSI	50
C	RHOC(1)=68.6*0.075=5.145	DNSI	51
C	RHOC(2)=80.0*0.541=43.28	DNSI	52
C	RHOC(3)=17.8*542=9.6476	DNSI	53
C		DNSI	54
C		DNSI	55
C	MASFRC(1)=0.4	DNSI	56
C	MASFRC(2)=0.25	DNSI	57
C	MASFRC(3)=0.35	DNSI	58
C		DNSI	59
C		DNSI	60
C		DNSI	61
C	-----INITIALIZE	DNSI	62
C		DNSI	63
C		DNSI	64
C		DNSI	65
C	XN(I,J)=ORDER OF THE KINETIC EXPRESSION.	DNSI	66
C		DNSI	67
	DO3J=1,NREACT	DNSI	68

3 READ 4,I,A(J),E(J),XN(I,J)	DNSI 69
4 FORMAT(4X,I6,3E10.8)	DNSI 70
READ 5,(RHOI(I),RHOC(I),MASFRC(I),I=1,COMPST)	DNSI 71
5 FORMAT(3E10.4)	DNSI 72
C	DNSI 73
C	DNSI 74
C    RHOI(I)=INITIAL DENSITY OF COMPOSITE I	DNSI 75
C    RHOC(I)=RESIDUAL DENSITY OF COMPOSITE I	DNSI 76
C    RHOT(I)=DENSITY OF THE COMPOSITE I AT ANY TEMPERATURE	DNSI 77
C	DNSI 78
C	DNSI 79
C	DNSI 80
C-----LET RHOT(I)=RHOI(I) AS INITIAL CONDITION	DNSI 81
C	DNSI 82
C	DNSI 83
DO 6 I=1,COMPST	DNSI 84
RHOC(I)=RHOC(I)+0.001*RHOC(I)	DNSI 85
MASFLX(I)=0.	DNSI 86
6    RHOT(I)=RHOI(I)	DNSI 87
SUMVOL=0.	DNSI 88
DO 60 I=1,COMPST	DNSI 89
VOLUME(I)=MASFRC(I)/RHOT(I)	DNSI 90
60    SUMVOL=SUMVOL+VOLUME(I)	DNSI 91
DO 65 I=1,COMPST	DNSI 92
65    VOLFRC(I)=VOLUME(I)/SUMVOL	DNSI 93
RHO=1./SUMVOL	DNSI 94
RHOI=1./SUMVOL	DNSI 95
WTOTAL=RHOI*VR	DNSI 96
PRINT 66,RHO,WTOTAL	DNSI 97
66    FORMAT(1X,'INITIAL DENSITY OF COMPOSITE(LBS/FT**3)='F10.5,2X,	DNSI 98
1'WTOTAL(LBS/FT**2-SEC)='E15.7/)	DNSI 99
7    RRR=1000./(R*T)	DNSI 100
RHOPRV=RHO	DNSI 101
DO 9 I=1,COMPST	DNSI 102

SUM=0.	DNSI 103
DO 8 J=1,NREACT	DNSI 104
IF(XN(I,J).EQ.0.)GOTO8	DNSI 105
C	DNSI 106
C RATER(J)=SPECIFIC REACTION VELOCITY	DNSI 107
IF(RHOT(I).LE.RHOC(I))RHOT(I)=RHOC(I)	DNSI 108
RATER(J)=-RHOT(I)*((RHOT(I)-RHOC(I))/RHOI(I))**XN(I,J)*A(J)*EXP(-	DNSI 109
1E(J)*RRR)	DNSI 110
SUM=SUM+RATER(J)	DNSI 111
8 CONTINUE	DNSI 112
DRHODT(I)=SUM	DNSI 113
IF(RHOT(I).LE.RHOC(I))DRHODT(I)=0.	DNSI 114
9 CONTINUE	DNSI 115
PRINT 900,H,DELZ	DNSI 116
900 FORMAT(1X,' IN DENSITY      H='E15.7,' DELZ='E15.7)	DNSI 117
C	DNSI 118
C-----CONTROLLING STEP SIZE FOR STABILITY	DNSI 119
C	DNSI 120
TEST=0.	DNSI 121
DO 90 I=1,COMPST	DNSI 122
DRHO(I)=-DELZ*DRHODT(I)/VR	DNSI 123
90 TEST=AMAX1(TEST,DRHO(I))	DNSI 124
IF(TEST.GT.0.5)H=H/2.	DNSI 125
IF(TEST.LT..1)H=H*2.	DNSI 126
IF(H.GT.2.08E-4)H=2.08E-4	DNSI 127
C DELZ=STEP SIZE IN FEET	DNSI 128
DELZ=H	DNSI 129
RHO=0.	DNSI 130
W=0.	DNSI 131
DO10I=1,COMPST	DNSI 132
DELFLX(I)=-DELZ*DRHODT(I)	DNSI 133
C	DNSI 134
C DELFLX(I)=CHANGE IN MASS FLUX DUE TO A CHANGE IN THE	DNSI 135
C DENSITY OF THE COMPOSITES.	DNSI 136

C	RHOT(I)=RHOT(I)-DELFLX(I)/VR	DN SI 137
	RHOVOL(I)=RHOT(I)*VOLFRC(I)	DN SI 138
	RHO=RHO+RHOVOL(I)	DN SI 139
		DN SI 140
C	RHO=BULK DENSITY OF THE COMPOSITE	DN SI 141
	MASFLX(I)=MASFLX(I)+DELFLX(I)	DN SI 142
10	W=W+MASFLX(I)	DN SI 143
	W1=(RHOI1-RHO)*VR	DN SI 144
	W=W1	DN SI 145
	DO 100 I=1,COMPST	DN SI 146
100	MASFRC(I)=RHOVOL(I)/RHO	DN SI 147
	PRINT 11,RHO,DELZ,VR,T,W	DN SI 148
11	FORMAT(1X,'RHO(OVERALL DENSITY OF ='E10.4,' DELZ='E10.4,' V='E10.4,	DN SI 149
	1' T='E10.4,' W='E13.5)	DN SI 150
	PRINT 12	DN SI 151
12	FORMAT(8X,'VIRGIN MATERIAL'))	DN SI 152
	DO 14 I=1,COMPST	DN SI 153
	PRINT 13,I,RHOT(I),I,DRHODT(I),I,DRHO(I),I,MASFRC(I)	DN SI 154
13	FORMAT(1X,'RHOT('I1,')='E12.6,' DRODT('I1,')='E12.6,' DRHO('I1,')=	DN SI 155
	1'E12.6,' MASFRC('I1,')='E12.6)	DN SI 156
14	CONTINUE	DN SI 157
	RETURN	DN SI 158
	END	DN SI 159

	SUBROUTINE CHARPR	CHAR	1
C	CHARPR SUBROUTINE CALCULATES THE EFFECTIVE THERMAL	CHAR	2
C	CONDUCTIVITY AND HEAT CAPACITY OF THE CHAR.	CHAR	3
C		CHAR	4
C		CHAR	5
	COMMON/KF/CPS,CDO,DCDO,JCHAR,TC	CHAR	6
C	T=TEMPERATURE IN RANKINE	CHAR	7
C	TC=TEMPERATURE IN FARENHEIT	CHAR	8
C	CPS=HEAT CAPACITY OF CHAR(BTU/LB-OF)	CHAR	9
C	CDO=EFFECTIVE THERMAL CONDUCTIVITY(BTU/FT-SEC-OF)	CHAR	10
C	DCDO=RATE OF CHANGE OF CDO WITH TEMPERATURE	CHAR	11
	TC2=TC*TC	CHAR	12
	TC3=TC2*TC	CHAR	13
	IF(TC.GT.2500.)GOTO507	CHAR	14
	T=TC+459.7	CHAR	15
	CPS=0.43+3.6E-5*T-87.2E3/(T*T)	CHAR	16
	IF(TC.LT.1000.)CPS=0.39	CHAR	17
507	CPS=0.52	CHAR	18
	CDO=11.57E-5+5.3E-15*TC3	CHAR	19
	DCDO=15.9E-15*TC2	CHAR	20
	RETURN	CHAR	21
	END	CHAR	22

SUBROUTINE CPMIX(T,NN,CPMX)	CPMI	1
C	CPMI	2
C	CPMI	3
C-----THIS SUBROUTINE COMPUTES THE MOLAL HEAT CAPACITY	CPMI	4
C OF A NON-REACTING GAS. IT IS ONLY USE FOR THE	CPMI	5
C FROZEN FLOW CASE.	CPMI	6
C	CPMI	7
C	CPMI	8
COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),FI(30),	CPMI	9
1GI(30),AII(30),BII(30),CII(30),DII(30),EII(30),	CPMI	10
2FII(30),GII(30),TLOW(30)	CPMI	11
COMMON/KM/XMOL(30)	CPMI	12
DIMENSION CP(30)	CPMI	13
RR=1.98726	CPMI	14
C	CPMI	15
C CPMX=HEAT CAPCITY(BTU/LB-MOLE-OF)	CPMI	16
C	CPMI	17
C	CPMI	18
C	CPMI	19
C-----CALCULATE THE HEAT CAPACITY OF EACH INDIVIDUAL SPECIE.	CPMI	20
C	CPMI	21
C	CPMI	22
CPMX=0.	CPMI	23
DO 3 I=1,NN	CPMI	24
IF(T.GT.TLOW(I))GOTO1	CPMI	25
CP(I)=(AII(I)+(((EII(I)*T+DII(I))*T+CII(I))*T+BII(I))*T)*RR	CPMI	26
GOTO2	CPMI	27
1 CP(I)=(AI(I)+(((EI(I)*T+DI(I))*T+CI(I))*T+BI(I))*T)*RR	CPMI	28
2 CPMX=CPMX+CP(I)*XMOL(I)	CPMI	29
3 CONTINUE	CPMI	30
RETURN	CPMI	31
END	CPMI	32



	SUBROUTINE CHEMEQ	CHEM	1
C		CHEM	2
C		CHEM	3
C		CHEM	4
C	-----THIS SUBPROGRAM COMPUTES COMPLEX CHEMICAL EQUILIBRIUM	CHEM	5
C	FOR A MULTICOMPONENT, POLYPHASE SYSTEM BY FREE ENERGY	CHEM	6
C	MINIMIZATION. (J. CHEM. PHYS. VOL. 28, NO. 5, 751-58, MAY 1958).	CHEM	7
C		CHEM	8
C		CHEM	9
	COMMON/KA/S1(6),S2(6),S3(6),S4(6),S5(6),S6(6),A11(6),	CHEM	10
	1A22(6),A33(6),A44(6),A55(6),A66(6),AA(30,6),JCODE(6)	CHEM	11
	COMMON/K8/AI(30),BI(30),CI(30),DI(30),EI(30),FI(30),	CHEM	12
	1GI(30),AII(30),BII(30),CII(30),DII(30),EII(30),	CHEM	13
	2FII(30),GII(30),TLOW(30)	CHEM	14
	COMMON/KC/ICODE(30),Y(30),XMW(30)	CHEM	15
	COMMON/KCC/SPCIE1(30),SPCIE2(30),TABLE(353,25)	CHEM	16
	COMMON/KGG/FORT(30),CP(30)	CHEM	17
	COMMON/KEE/PL,RR,TZERO,EPS,KEY,NN,NQ,MM	CHEM	18
	COMMON/KI/WEPS,KPT3,KOUNT	CHEM	19
	COMMON/KJ/DELTK,TVAR	CHEM	20
	COMMON/KG/ENT(30),S(30),ENT1(30),T	CHEM	21
	COMMON/KNN/TFMAX	CHEM	22
	DIMENSION PERC(30),PERC1(30),XMOL(30),XMOL1(30)	CHEM	23
	DIMENSION X(30),FY(30),C(30),BB(8),FSUM(30),YSUM(30),	CHEM	24
	1XMASS(30),XLAM(30),FLUX(350,25),	CHEM	25
	2DFLUX(350,25),R(6,6),B(6,1),PI(6),DELT(30)	CHEM	26
C		CHEM	27
C		CHEM	28
C	PL=PRESSURE IN LBS/FT2	CHEM	29
C	RR=1.987(CAL/GM-MOLE-OK)	CHEM	30
C	TZERO=298.16 OK	CHEM	31
C	EPS=POROSITY OF THE MATRIX	CHEM	32
C	KEY=2 FOR EQUILIBRIUM FLOW	CHEM	33
C	NN=NUMBER OF GAS COMPONENTS	CHEM	34

C	NQ=NUMBER OF SOLID+GAS COMPONENTS	CHEM	35
C	TABLE(I,J)STORES THE VALUES OF THE TEMPERATURE(J=1)IN	CHEM	36
C	OK,THE HEAT ABSORBED OR RELEASED BY CHEMICAL REACTIONS	CHEM	37
C	(J=2)(BTU/FT**3-SEC),THE AVERAGE MOLECULAR WEIGHT OF THE	CHEM	38
C	MIXTURE(J=3),THE MASS FLOW RATE OF THE GASES(LBS/FT2-SEC),	CHEM	39
C	AND THE AVERAGE HEAT CAPACITY OF THE MIXTURE.	CHEM	40
C	FROM J=5 ON,THE VALUES OF MOLES,Y(I),OF EACH INDIVIDUAL	CHEM	41
C	ARE STORED. I IS THE NUMBER OF TEMPERATURE POINTS	CHEM	42
C		CHEM	43
	W1=WEPS/EPS	CHEM	44
	W=WEPS/EPS	CHEM	45
	XT=TVAR	CHEM	46
	CRIT=0.0001	CHEM	47
	TMAX=(TFMAX+459.69)/1.8	CHEM	48
	TINC=(TMAX-XT)/346.	CHEM	49
	IF(TINC.LT.7.5)TINC=7.5	CHEM	50
	TINC=200.	CHEM	51
	TMAX=TMAX+4.*TINC	CHEM	52
	READ 7,IPRINT	CHEM	53
7	FORMAT(I1)	CHEM	54
	NS=NQ	CHEM	55
	NC=NN	CHEM	56
C		CHEM	57
C	XT=INITIAL TEMPERATURE(OK)	CHEM	58
C	TMAX=FINAL TEMPERATURE(OK)	CHEM	59
C	TINC=INCREMENT OF TEMPERATURE	CHEM	60
C	CRIT=CRITERIA FOR CONVERGENCE	CHEM	61
C	KEY=2(EQUILIBRIUM)	CHEM	62
C		CHEM	63
	MA=1	CHEM	64
	M=MA	CHEM	65
C		CHEM	66
C	-----CALCULATE THE SIZE OF THE MATRIX R.	CHEM	67
C		CHEM	68

NA=MM+1+NQ-NN	CHEM 69
N=NA	CHEM 70
P=PL/2160.	CHEM 71
KPT=0	CHEM 72
C	CHEM 73
C KPT COUNTS THE NUMBER OF TEMPERATURE POINTS	CHEM 74
C	CHEM 75
MAXNT=100	CHEM 76
C MAXNT=MAXIMUM NUMBER OF ITERATIONS ALLOWED	CHEM 77
C BEFORE INCREASING CRIT(CRIT=CRITERIA FOR CONVERGENCE)	CHEM 78
KCODE=0	CHEM 79
C KCODE=0(NO SOLIDS ),KCODE=1(SOLIDS ARE ASSUMED PRESENT)	CHEM 80
T=XT	CHEM 81
KOS=NQ+5	CHEM 82
C	CHEM 83
C KOS IS THE TOTAL NUMBER OF VARIABLES STORED	CHEM 84
C IN TABLE(I,J)(J=1...KOS)	CHEM 85
C ENT(I)=HEAT OF FORMATION OF SPECIE I	CHEM 86
C FORT(I)=FREE ENERGY FUNCTION(F/RT)	CHEM 87
C FORT IS CALCULATED IN SUBROUTINE FRNERG	CHEM 88
LL=NN+1	CHEM 89
XBETA=CRIT	CHEM 90
C	CHEM 91
C-----CALCULATE THE GRAM-ATOMS OF EACH ELEMENT,BB(J).	CHEM 92
C BB(J)IS THE MATERIAL BALANCE CONSTRAINT ON THE	CHEM 93
C FREE ENERGY EQUATION.	CHEM 94
C	CHEM 95
DO320J=1,MM	CHEM 96
BB(J)=0.	CHEM 97
DO 320 I=1,NQ	CHEM 98
BB(J)=BB(J)+AA(I,J)*Y(I)	CHEM 99
320 CONTINUE	CHEM 100
DO433I=1,NQ	CHEM 101
IF(ICODE(I).EQ.0)GOTO433	CHEM 102

KCODE=1	CHEM 103
433 CONTINUE	CHEM 104
C	CHEM 105
C-----TEST TO DETERMINE WHETHER THERE ARE SOLIDS IN THE	CHEM 106
C SYSTEM OF SPECIES ASSUMED.	CHEM 107
C	CHEM 108
500 IF(IPRINT .EQ. 0) GO TO 501	CHEM 109
PRINT4	CHEM 110
4 FORMAT(1H1,20X,5HFC/RT,13X,12HINITIAL Y(I))	CHEM 111
C	CHEM 112
C-----CALL THE FREE ENERGY SUBPROGRAM	CHEM 113
C	CHEM 114
501 NT=1	CHEM 115
CALL FRNERG(T,NQ)	CHEM 116
C	CHEM 117
C-----THE ABOVE SUBPROGRAM CALCULATES THE FREE ENRGY FUNCTION FORT.	CHEM 118
C	CHEM 119
IF(IPRINT .EQ. 0) GO TO 300	CHEM 120
DO206I=1,NQ	CHEM 121
206 PRINT14,I,SPCIE1(I),SPCIE2(I),FORT(I),Y(I),XMW(I)	CHEM 122
14 FORMAT(1X,I2,2X,2A3,3E20.7)	CHEM 123
300 YBAR=0.0	CHEM 124
DO50I=1,NN	CHEM 125
C	CHEM 126
C	CHEM 127
C YBAR IS THE TOTAL NUMBER OF MOLES OF GAS SPECIES	CHEM 128
C	CHEM 129
50 YBAR=YBAR+Y(I)	CHEM 130
DO10I=1,NN	CHEM 131
C(I)=FORT(I)+ALOG(P)	CHEM 132
FAC=Y(I)/YBAR	CHEM 133
IF(FAC.LT.1.E-73)FAC=1.E-73	CHEM 134
C	CHEM 135
C-----CALCULATE THE FREE ENERGY PARAMETER OF THE GAS SPECIES	CHEM 136

C	TO BE MINIMIZE	CHEM 137
C		CHEM 138
	FY(I)=Y(I)*(C(I)+ALOG(FAC))	CHEM 139
10	CONTINUE	CHEM 140
	IF(KCODE.EQ.0)GOTO111	CHEM 141
C		CHEM 142
C		CHEM 143
C	-----IF THERE ARE NO SOLIDS PROCEED TO STATEMENT 111	CHEM 144
C		CHEM 145
C		CHEM 146
C	-----CALCULATION OF THE FREE ENERGY PARAMENTER FOR SOLIDS	CHEM 147
C		CHEM 148
	DO 11 I=LL,NQ	CHEM 149
	FY(I)=Y(I)*FORT(I)	CHEM 150
11	CONTINUE	CHEM 151
C		CHEM 152
C	-----FROM STATEMENT 111 TO 1050 OPERATIONS ARE PERFORMED TO CONSTRUCT	CHEM 153
C	THE R MATRIX AND THE B VECTOR	CHEM 154
C		CHEM 155
C		CHEM 156
111	DO30J=1,MM	CHEM 157
	DO30K=1,MM	CHEM 158
	SUM=0.	CHEM 159
	DO20I=1,NN	CHEM 160
20	SUM=SUM+AA(I,J)*AA(I,K)*Y(I)	CHEM 161
	R(J,K)=SUM	CHEM 162
30	CONTINUE	CHEM 163
	GSUM1=0.	CHEM 164
	DO 1022 I=1,NQ	CHEM 165
	GSUM1=GSUM1+FY(I)	CHEM 166
1022	CONTINUE	CHEM 167
3000	JJ=MM+1	CHEM 168
	DO 103 K=1,MM	CHEM 169
	SUM=0.	CHEM 170

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DO 101 I=1,NN
101 SUM=SUM+AA(I,K)*Y(I)
   R(K,JJ)=SUM
   R(JJ,K)=SUM
103 CONTINUE
   KL=NS-NC+JJ
   DO 1044 J=JJ,KL
   DO 1045 K=JJ,KL
1045 R(J,K)=0.0
1044 CONTINUE
   DO70J=1,MM
   SUM=0.
   DO130I=1,NN
130 SUM=SUM+AA(I,J)*FY(I)
   70 B(J,1)=SUM+BB(J)
   SUM=0.
   DO80I=1,NN
80 SUM=SUM+FY(I)
   B(JJ,1)=SUM
   IF(KCODE.EQ.0)GOTO1050
   KK=MM+1
   DO 29 I=LL,NQ
   KK=KK+1
   DO 29 J=1,MM
   R(J,KK)=AA(I,J)
   R(KK,J)=R(J,KK)
29 CONTINUE
   KM=MM+1
   DO 1053 I=LL,NQ
   KM=KM+1
1053 B(KM,1)=FORT(I)
1050 CONTINUE
   IF(KCODE.EQ.0)R(JJ,JJ)=0.

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CHEM 171
CHEM 172
CHEM 173
CHEM 174
CHEM 175
CHEM 176
CHEM 177
CHEM 178
CHEM 179
CHEM 180
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CHEM 201
CHEM 202
CHEM 203
CHEM 204

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C

C-----MATRIX INVERSION IS CALLED TO SOLVE THE SET OF SIMULTANEOUS	CHEM 205
C     LINEARIZED EQUATIONS.	CHEM 206
C	CHEM 207
C	CHEM 208
CALL MATINV(R,NA,B,MA)	CHEM 209
C	CHEM 210
C	CHEM 211
C-----FROM THE SOLUTION OF THE MATRIX THE VALUES OF THE LAGRANGIAN	CHEM 212
C     MULTIPLIERS AND THE MOLES OF THE SOLID SPECIES ARE OBTAINED	CHEM 213
C	CHEM 214
C	CHEM 215
DO100I=1,JJ	CHEM 216
100 PI(I)=B(I,M)	CHEM 217
U=PI(JJ)	CHEM 218
XBAR=U*YBAR	CHEM 219
IF(KCODE.EQ.0)GOTO59	CHEM 220
KK=MM+2	CHEM 221
LW=LL	CHEM 222
DO 1002 J=KK,KL	CHEM 223
X(LW)=B(J,M)	CHEM 224
1002 LW=LW+1	CHEM 225
59 DO60I=1,NN	CHEM 226
60 FSUM(I)=-FY(I)+(Y(I)/YBAR)*XBAR	CHEM 227
DO110I=1,NN	CHEM 228
PSUM=0.	CHEM 229
DO120J=1,MM	CHEM 230
120 PSUM=PSUM+PI(J)*AA(I,J)	CHEM 231
YSUM(I)=PSUM*Y(I)	CHEM 232
C	CHEM 233
C-----CALCULATE THE MOLES OF GASEOUS SPECIES	CHEM 234
C	CHEM 235
110 X(I)=FSUM(I)+YSUM(I)	CHEM 236
C	CHEM 237
C-----CALCUALTE THE CONVERGENCE PARAMENTE XLAMBD	CHEM 238

C	XLAMBD=1.0	CHEM 239
	DD 86 I=1,NQ	CHEM 240
	DELT(I)=X(I)-Y(I)	CHEM 241
	IF(DELT(I).GE.0.)GOTO86	CHEM 242
	IF(X(I).GT.0.)GOTO86	CHEM 243
	XLAM(I)=-Y(I)/DELT(I)	CHEM 244
	XLAMBD=AMIN1(XLAMBD,XLAM(I))	CHEM 245
	XLAMBD=C.99*XLAMBD	CHEM 246
86	CONTINUE	CHEM 247
	XLAM1=XLAMBD	CHEM 248
	IF(XLAM1.EQ.0.)XLAM1=1.E-5	CHEM 249
	DEBAR=0.	CHEM 250
	DD87I=1,NN	CHEM 251
87	DEBAR=DEBAR+DELT(I)	CHEM 252
C		CHEM 253
C		CHEM 254
C	-----DETERMINE THE SIZE OF THE UNIT VECTOR XLAMBD.	CHEM 255
C	APPLY THE CORRECTIONS TO OBTAIN A NEW SET OF ESTIMATES FOR THE	CHEM 256
C	NEXT ITERATION. WHEN THE VALUE OF XLAMBD IS VERY SMALL SET THE	CHEM 257
C	VALUES OF Y(I) EQUAL TO X(I) TO AVOID USING THE SAME VALUES OF	CHEM 258
C	Y(I) AS WAS USED IN THE PREVIOUS ITERATION	CHEM 259
C		CHEM 260
C		CHEM 261
C		CHEM 262
C		CHEM 263
C	-----CALCUALTE THE FREE NERGY GRADIENT DFDL. IF IT IS POSITIVE	CHEM 264
C	REDUCE THE VALUE OF XLAMBD UNTIL DFDL IS NEGATIVE.	CHEM 265
C		CHEM 266
93	DFDL=0.	CHEM 267
	DD88I=1,NQ	CHEM 268
	IF(ICODE(I).EQ.1)GOTO83	CHEM 269
96	FAC=(Y(I)+XLAMBD*DELT(I))/(YBAR+XLAMBD*DEBAR)	CHEM 270
98	IF(FAC.GT.0.)GOTO82	CHEM 271
991	XLAMBD=.9*XLAMBD	CHEM 272



IF(XLAMBD.GT.1.0E- 6)GOTO96	CHEM 273
IF(FAC.LT.1.E-73)FAC=1.E-73	CHEM 274
82 DFDL=DFDL+DELT(I)*(C(I)+ALOG(FAC))	CHEM 275
GOTO88	CHEM 276
83 DFDL=DFDL+DELT(I)*FORT(I)	CHEM 277
88 CONTINUE	CHEM 278
IF(DFDL.LT.0.000)GOTO89	CHEM 279
XLAMBD=.9*XLAMBD	CHEM 280
IF(XLAMBD.GT.1.0E- 6)GOTO93	CHEM 281
C	CHEM 282
C-----CALCULATE THE NEW AND IMPROVED VALUE OF THE MOLES OF THE SPECIES.	CHEM 283
C	CHEM 284
89 DO76I=1,NQ	CHEM 285
IF(XLAMBD.GT.1.E-6)GOTO90	CHEM 286
IF(DFDL.LT.0.)GOTO90	CHEM 287
IF(XLAM1.LT.1.E-6)XLAM1=1.E-6	CHEM 288
Y(I)=Y(I)+XLAM1*DELT(I)*.1	CHEM 289
GOTO900	CHEM 290
90 CONTINUE	CHEM 291
Y(I)=Y(I)+XLAMBD*DELT(I)	CHEM 292
900 CONTINUE	CHEM 293
IF(Y(I).LT.0.)Y(I)=1.E-73	CHEM 294
76 CONTINUE	CHEM 295
SUMY=0.	CHEM 296
SUM=0.	CHEM 297
DO370I=1,NN	CHEM 298
370 SUMY=SUMY+Y(I)	CHEM 299
DO371I=LL,NQ	CHEM 300
371 SUM=SUM+Y(I)	CHEM 301
SUMY1=SUMY+SUM	CHEM 302
DO340I=1,NQ	CHEM 303
XMOL1(I)=Y(I)/SUMY1	CHEM 304
PERC1(I)=XMOL1(I)*100.	CHEM 305
XMOL(I)=Y(I)/SUMY	CHEM 306

340	PERC(I)=XMOL(I)*100.	CHEM 307
	GSUM2=0.	CHEM 308
	DO342I=1,NQ	CHEM 309
	IF(ICODE(I).EQ.1)GOTO341	CHEM 310
	FAC=XMOL(I)	CHEM 311
	IF(FAC.LT.1.E-73)FAC=1.E-73	CHEM 312
	FY(I)=Y(I)*(C(I)+ALOG(FAC))	CHEM 313
	GSUM2=GSUM2+FY(I)	CHEM 314
	GOTO342	CHEM 315
341	FY(I)=Y(I)*FORT(I)	CHEM 316
	GSUM2=GSUM2+FY(I)	CHEM 317
342	CONTINUE	CHEM 318
350	BETA=0.	CHEM 319
	DO85I=1,NQ	CHEM 320
C		CHEM 321
C-----	CHECK IF THE MINIMUM HAS BEEN REACHED	CHEM 322
C		CHEM 323
85	BETA=BETA+ABS(DELT(I))	CHEM 324
	RESTA=1.0000000-U	CHEM 325
	IF(ABS(RESTA).LT.XBETA)GOTO800	CHEM 326
	IF(NT.GE.MAXNT)GOTO600	CHEM 327
	NT=NT+1	CHEM 328
	GOTO300	CHEM 329
600	XBETA=XBETA+0.001	CHEM 330
	MAXNT=MAXNT+10	CHEM 331
	NT=NT+1	CHEM 332
	GOTO300	CHEM 333
C*****		CHEM 334
C*****		CHEM 335
C-----	CONVERGENCE HAS BEEN ACHIEVED	* CHEM 336
C*****		CHEM 337
C*****		CHEM 338
800	IF(IPRINT.EQ.0) GO TO 1802	CHEM 339
	PRINT16,NT,U	CHEM 340

16	FORMAT(//1X,'NT = NO. OF ITERATIONS REQUIRED ='15,5X,	CHEM 341
	1'U=X/Y='F15.7/ )	CHEM 342
	PRINT2189,(J,BB(J),J=1,MM)	CHEM 343
2189	FORMAT(1X,'BB('11,')='F15.7)	CHEM 344
	PRINT201,BETA	CHEM 345
201	FORMAT( /1X,'BETA='F15.7/ )	CHEM 346
	PRINT202,GSUM2	CHEM 347
202	FORMAT(1X,'FREE ENERGY FY(I) OF THE SYSTEM AT EQUILIBRIUM'F15.7)	CHEM 348
	PRINT203,P,T	CHEM 349
203	FORMAT( /1X,'PRESSURE(ATM)='F10.4,5X,'TEMP(OK)='F13.6/ )	CHEM 350
1802	XMWGAS=0.	CHEM 351
	DO811=1,NN	CHEM 352
C		CHEM 353
C-----	CALCULATE THE AVERAGE MOLECULAR WEIGHT OF THE GAS, XMWGAS	CHEM 354
C		CHEM 355
81	XMWGAS=XMWGAS+XMOL(I)*XMW(I)	CHEM 356
	DO1911=1,NQ	CHEM 357
191	XMASS(I)=XMW(I)*XMOL(I)/XMWGAS	CHEM 358
	CPMX=0.	CHEM 359
	DO7811=1,NN	CHEM 360
781	CPMX=CPMX+CP(I)*XMOL(I)	CHEM 361
	IF(IPRINT .EQ. 0) GO TO 1803	CHEM 362
	PRINT 18,CPMX,W	CHEM 363
18	FORMAT( /1X,'HEAT CAPACITY OF THE MIXTURE'/1X,'IN CALORIES PER GRACHEM	CHEM 364
	1M MOLE ='F10.5,10X,'MASS FLUX(LBS/FT2SEC)='F10.5)	CHEM 365
	PRINT17, XMWGAS	CHEM 366
17	FORMAT( /1X,'MOLECULAR WEIGHT OF THE GAS MIXTURE='F8.5)	CHEM 367
1803	XBETA=CRIT	CHEM 368
	KPT=KPT+1	CHEM 369
C		CHEM 370
C		CHEM 371
C-----	REDIFINE MOLE BASIS. THIS OPERATION IS PERFORMED AFTER	CHEM 372
C	THE FIRST EQUILIBRIUM CALCULATION. THIS IS DONE TO MAKE	CHEM 373
C	THE MOLES OF Y(I) CALCULATED BASED ON ONE MOLE OF VIR-	CHEM 374

C PLASTIC COMPOSITE COMPATIBLE WITH THE ACTUAL NUMBER  
 C OF MOLES FLOWING THROUGH THE POROUS MATRIX. THIS OPERA-  
 C TION IS PERFORMED ONLY ONCE.

C IF(T.NE.XT)GOTO823

C  
 C-----PROPORTION THE MOLES OF FLOWING GASES IN DIRECT  
 C RELATION TO THEIR EQUILIBRIUM MOLE FRACTION.

C RIN=0.

C SUM=0.

C DO821I=1,NQ

C IF(ICODE(I).EQ.1)GOTO8210

C Y(I)=W/XMWGAS\*XMOL(I)

C SUM=SUM+Y(I)

C GOTO821

8210 Y(I)=XMOL(I)\*SUM

C RIN=RIN+XMOL(I)\*XMW(I)/XMWGAS

821 CONTINUE

C  
 C-----RIN=THE RATIO OF THE MASS OF THE SOLID MATRIX  
 C TO THE MASS OF THE FLOWING GASES AT THE  
 C PREVIOUS TEMPERATURE STATION.

C  
 C  
 C-----ROUT=THE SAME RATIO AT AN INCREMENT OF TEMPERA-  
 C TURE DOWN THE FLOW FIELD.  
 C TO INITIALIZE, ROUT IS SET EQUAL TO RIN.

C ROUT=RIN

C  
 C-----RECOMPUTE THE MATERIAL BALANCE CONSTRAINTS.

CHEM 375  
 CHEM 376  
 CHEM 377  
 CHEM 378  
 CHEM 379  
 CHEM 380  
 CHEM 381  
 CHEM 382  
 CHEM 383  
 CHEM 384  
 CHEM 385  
 CHEM 386  
 CHEM 387  
 CHEM 388  
 CHEM 389  
 CHEM 390  
 CHEM 391  
 CHEM 392  
 CHEM 393  
 CHEM 394  
 CHEM 395  
 CHEM 396  
 CHEM 397  
 CHEM 398  
 CHEM 399  
 CHEM 400  
 CHEM 401  
 CHEM 402  
 CHEM 403  
 CHEM 404  
 CHEM 405  
 CHEM 406  
 CHEM 407  
 CHEM 408

DO79J=1,MM	CHEM 409
BB(J)=0.	CHEM 410
DO79I=1,NQ	CHEM 411
79 BB(J)=BB(J)+AA(I,J)*Y(I)	CHEM 412
GOTO171	CHEM 413
823 ROUT=0.	CHEM 414
DO824I=LL,NQ	CHEM 415
824 ROUT=ROUT+XMOL(I)*XMW(I)/XMWGAS	CHEM 416
RATIO=(1.+RIN)/(1.+ROUT)	CHEM 417
C	CHEM 418
C RATIO IS THE FRACTION GAIN OR LOSS OF SOLID	CHEM 419
C MATERIAL BY THE FLOWING GASES.	CHEM 420
C	CHEM 421
W=W*RATIO	CHEM 422
RIN=ROUT	CHEM 423
171 TABLE(KPT,1)=T	CHEM 424
TABLE(KPT,3)=XMWGAS	CHEM 425
TABLE(KPT,4)=W	CHEM 426
PRINT 172,W,T	CHEM 427
172 FORMAT(1X,'W='E15.7,E20.7)	CHEM 428
TABLE(KPT,5)=CPMX	CHEM 429
C	CHEM 430
C	CHEM 431
C-----CALCULATION AND STORAGE OF THE INDIVIDUAL MASS	CHEM 432
C FLUXES AT EVERY TEMPERATURE IN VARIABLE FLUX(J,I)	CHEM 433
C FOLLOWS. THESE STORED VALUES ARE USED SUBSEQUENT-	CHEM 434
C LY TO COMPUTE THE DERATIVE OF FLUX(J,I)WITH TEM-	CHEM 435
C PERATURE, WHICH IS DFLUX(J,I). THIS VARIABLE IS	CHEM 436
C USED TO COMPUTE A VARIABLE CALL REACT, WHICH ACCOUNTS	CHEM 437
C FOR THE HEAT EFFECTS OF THE CHEMICAL REACTIONS.	CHEM 438
C NOTICE THAT THE KFACT TERM HAS TO BE MULTIPLIED BY	CHEM 439
C THE GRADIENT OF TEMPERATURE WITH DISTANCE. THIS OPE-	CHEM 440
C RATION IS PERFORMED IN THE MAIN PROGRAM.	CHEM 441
C	CHEM 442

C	IF(IPRINT .EQ. 0) GO TO 1804	CHEM 443
	PRINT204	CHEM 444
204	FORMAT(/6X,'I',21X,'Y(I)',9X,'MOLE FRACTION',5X,	CHEM 445
	1'MASS FRACTION')	CHEM 446
1804	DO1712I=1,NQ	CHEM 447
	FLUX(KPT,I)=W*XMASS(I)	CHEM 448
	IF(IPRINT .EQ. 0) GO TO 1712	CHEM 449
	PRINT19,I,SPCIE1(I),SPCIE2(I),Y(I),XMOL(I),XMASS(I),FLUX(KPT,I)	CHEM 450
1712	CONTINUE	CHEM 451
19	FORMAT(1X,I6,3X,2A3,2X,4E18.7)	CHEM 452
	DO1713I=6,KOS	CHEM 453
	II=I-5	CHEM 454
C		CHEM 455
C	THE UNITS OF FLUX(KPT,I) ARE LBS/FT2-SEC.	CHEM 456
C		CHEM 457
1713	TABLE(KPT,I)=XMOL(II)	CHEM 458
	IF(T.GE.TMAX)GOTO333	CHEM 459
	T=T+TINC	CHEM 460
	GOTO500	CHEM 461
C		CHEM 462
C-----	THE MOLE FRACTIONS AT EVERY TEMPERATURE UP TO TMAX	CHEM 463
C	HAVE BEEN STORED. THESE STORED VALUES WILL NOW BE	CHEM 464
C	USED TO COMPUTE THE DERIVATIVE OF FLUX. THAT IS, THE	CHEM 465
C	RATE OF CHANGE OF THE MASS FLOW RATE WITH TEMPERATURE.	CHEM 466
C	THIS RATE OF CHANGE WILL BE STORED IN VARIABLE DFLUX(J,I).	CHEM 467
C	THE UNITS OF DFLUX(J,I) ARE, LBS/FT2-SEC OK	CHEM 468
C		CHEM 469
333	KPT3=KPT-3	CHEM 470
	TINC60=1./(60.*TINC)	CHEM 471
	KOUNT=2	CHEM 472
	DO1717J=1,KPT3	CHEM 473
	DO1716I=1,NQ	CHEM 474
	IF(J.GT.2)GOTO1715	CHEM 475
		CHEM 476

IF(J.GT.1)GOTO1714	CHEM 477
DFLUX(J,I)=(1./(60.*TINC))*(-137.*FLUX(J,I)+300.*FLUX(J+1,I)	CHEM 478
1-300.*FLUX(J+2,I)+200.*FLUX(J+3,I)-75.*FLUX(J+4,I)	CHEM 479
2+12.*FLUX(J+5,I))	CHEM 480
GOTO1716	CHEM 481
1714 DFLUX(J,I)=TINC60*(-12.*FLUX(J-1,I)-65.*FLUX(J,I)+120.*FLUX(J+1,I)	CHEM 482
1-60.*FLUX(J+2,I)+20.*FLUX(J+3,I)-3.*FLUX(J+4,I))	CHEM 483
GO TO 1716	CHEM 484
1715 DFLUX(J,I)=TINC60*(3.*FLUX(J-2,I)-30.*FLUX(J-1,I)-20.*FLUX(J,I)	CHEM 485
1+60.*FLUX(J+1,I)-15.*FLUX(J+2,I)+2.*FLUX(J+3,I))	CHEM 486
1716 CONTINUE	CHEM 487
1717 CONTINUE	CHEM 488
C	CHEM 489
C-----CALCULATE THE HEAT TERM NECESSARY FOR GROUP	CHEM 490
C	CHEM 491
C IN THE MAIN PROGRAM.	CHEM 492
DO1722J=1,KPT3	CHEM 493
HEAT=0.	CHEM 494
PRINT 1718,J	CHEM 495
1718 FORMAT(1X,'J='I3/)	CHEM 496
PRINT 1719,(DFLUX(J,I),I=1,NQ)	CHEM 497
1719 FORMAT(1X,8E15.7)	CHEM 498
T=TABLE(J,1)	CHEM 499
CALL THERM1	CHEM 500
DO1721I=1,NQ	CHEM 501
IF(I.LE.NN)GOTO1720	CHEM 502
HEAT=HEAT+DFLUX(J,I)*ENT(I)*(1.-EPS)/XMW(I)	CHEM 503
GOTO1721	CHEM 504
1720 HEAT=HEAT+DFLUX(J,I)*ENT(I)*EPS/XMW(I)	CHEM 505
1721 CONTINUE	CHEM 506
1722 TABLE(J,2)=HEAT	CHEM 507
C THE UNITS OF HEAT ARE BTU/FT2-SEC OF	CHEM 508
RETURN	CHEM 509
END	CHEM 510

	SUBROUTINE FRNERG(T,NQ)	FRNE	1
C		FRNE	2
C	THIS SUBPROGRAM CALCULATES THE FREE ENERGY FUNCTION	FRNE	3
C	AND THE HEAT CAPACITY OF EACH INDIVIDUAL SPECIE.	FRNE	4
	COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),FI(30),GI(30),	FRNE	5
	1AII(30),BII(30),CII(30),DII(30),EII(30),FII(30),GII(30),	FRNE	6
	2TLOW(30)	FRNE	7
	COMMON/KGG/FORT(30),CP(30)	FRNE	8
	DO2I=1,NQ	FRNE	9
	IF(T.GT.TLOW(I))GOTO1	FRNE	10
	FORT(I)=AII(I)*(1.-ALOG(T))-((((EII(I)/20.)*T+DII(I)/12.)*T+	FRNE	11
	1CII(I)/6.)*T+BII(I)/2.)*T+FII(I)/T-GII(I)	FRNE	12
	CP(I)=AII(I)+(((EII(I)*T+DII(I))*T+CII(I))*T+BII(I))*T	FRNE	13
	GOTO2	FRNE	14
1	FORT(I)=AI(I)*(1.-ALOG(T))-((((EI(I)/20.)*T+DI(I)/12.)*T+	FRNE	15
	1CI(I)/6.)*T+BI(I)/2.)*T+FI(I)/T-GI(I)	FRNE	16
	CP(I)=AI(I)+(((EI(I)*T+DI(I))*T+CI(I))*T+BI(I))*T	FRNE	17
2	CONTINUE	FRNE	18
	RETURN	FRNE	19
	END	FRNE	20



C	SUBROUTINE MATINV(A,N,B,M)	MATI	1
C		MATI	2
C		MATI	3
C		MATI	4
C		MATI	5
C	MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS	MATI	6
C		MATI	7
C		MATI	8
	DIMENSION A(6,6),B(6,1),IPIVOT(6),INDEX(6,2)	MATI	9
	EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUM), (AMAX,T,SWAP)	MATI	10
C		MATI	11
C	INITIALIZATION	MATI	12
C		MATI	13
	5 ISCALE=0	MATI	14
	6 R1=10.0**18	MATI	15
	7 R2=1.0/R1	MATI	16
	10 DETERM=1.0	MATI	17
	15 DO 20 J=1,N	MATI	18
	20 IPIVOT(J)=0	MATI	19
	30 DO 550 I=1,N	MATI	20
C		MATI	21
C	SEARCH FOR PIVOT ELEMENT	MATI	22
C		MATI	23
	40 AMAX=0.0	MATI	24
	45 DO 105 J=1,N	MATI	25
	50 IF (IPIVOT(J)-1)60,105,60	MATI	26
	60 DO 100 K=1,N	MATI	27
	70 IF (IPIVOT(K)-1)80,100,740	MATI	28
	80 IF (ABS(AMAX)-ABS(A(J,K)))85,100,100	MATI	29
	85 IROW=J	MATI	30
	90 ICOLUM=K	MATI	31
	95 AMAX=A(J,K)	MATI	32
	100 CONTINUE	MATI	33
	105 CONTINUE	MATI	34

IF (AMAX)110,106,110	MATI 35
106 DETERM=0.0	MATI 36
ISCALE=0	MATI 37
GO TO 740	MATI 38
110 IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1	MATI 39
C	MATI 40
C INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL	MATI 41
C	MATI 42
130 IF (IROW-ICOLUM)140,260,140	MATI 43
140 DETERM=-DETERM	MATI 44
150 DO 200 L=1,N	MATI 45
160 SWAP=A(IROW,L)	MATI 46
170 A(IROW,L)=A(ICOLUM,L)	MATI 47
200 A(ICOLUM,L)=SWAP	MATI 48
205 IF(M)260,260,210	MATI 49
210 DO 250 L=1,M	MATI 50
220 SWAP=B(IROW,L)	MATI 51
230 B(IROW,L)=B(ICOLUM,L)	MATI 52
250 B(ICOLUM,L)=SWAP	MATI 53
260 INDEX(I,1)=IROW	MATI 54
270 INDEX(I,2)=ICOLUM	MATI 55
310 PIVOT=A(ICOLUM,ICOLUM)	MATI 56
C	MATI 57
C SCALE THE DETERMINANT	MATI 58
C	MATI 59
1000 PIVOTI=PIVOT	MATI 60
1005 IF(ABS(DETERM)-R1)1030,1010,1010	MATI 61
1010 DETERM=DETERM/R1	MATI 62
ISCALE=ISCALE+1	MATI 63
IF(ABS(DETERM)-R1)1060,1020,1020	MATI 64
1020 DETERM=DETERM/R1	MATI 65
ISCALE=ISCALE+1	MATI 66
GO TO 1060	MATI 67
1030 IF(ABS(DETERM)-R2)1040,1040,1060	MATI 68

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1040 DETERM=DETERM*R1
      ISCALE=ISCALE-1
      IF(ABS(DETERM)-R2)1050,1050,1060
1050 DETERM=DETERM*R1
      ISCALE=ISCALE-1
1060 IF(ABS(PIVOTI)-R1)1090,1070,1070
1070 PIVOTI=PIVOTI/R1
      ISCALE=ISCALE+1
      IF(ABS(PIVOTI)-R1)320,1080,1080
1080 PIVOTI=PIVOTI/R1
      ISCALE=ISCALE+1
      GO TO 320
1090 IF(ABS(PIVOTI)-R2)2000,2000,320
2000 PIVOTI=PIVOTI*R1
      ISCALE=ISCALE-1
      IF(ABS(PIVOTI)-R2)2010,2010,320
2010 PIVOTI=PIVOTI*R1
      ISCALE=ISCALE-1
320 DETERM=DETERM*PIVOTI
C
C      DIVIDE PIVOT ROW BY PIVOT ELEMENT
C
330 A(ICOLUM,ICOLUM)=1.0
340 DO 350 L=1,N
350 A(ICOLUM,L)=A(ICOLUM,L)/PIVOT
355 IF(M) 380,380,360
360 DO 370 L=1,M
370 B(ICOLUM,L)=B(ICOLUM,L)/PIVOT
C
C      REDUCE NON-PIVOT ROWS
C
380 DO 550 L1=1,N
390 IF(L1-ICOLUM)400,550,400
400 T=A(L1,ICOLUM)

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MATI 69
MATI 70
MATI 71
MATI 72
MATI 73
MATI 74
MATI 75
MATI 76
MATI 77
MATI 78
MATI 79
MATI 80
MATI 81
MATI 82
MATI 83
MATI 84
MATI 85
MATI 86
MATI 87
MATI 88
MATI 89
MATI 90
MATI 91
MATI 92
MATI 93
MATI 94
MATI 95
MATI 96
MATI 97
MATI 98
MATI 99
MATI 100
MATI 101
MATI 102

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420 A(L1,ICOLUM)=0.0
430 DO 450 L=1,N
450 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T
455 IF(M) 550,550,460
460 DO 500 L=1,M
500 B(L1,L)=B(L1,L)-B(ICOLUM,L)*T
550 CONTINUE

C
C   INTERCHANGE COLUMNS
C
600 DO 710 I=1,N
610 L=N+1-I
620 IF(INDEX(L,1)-INDEX(L,2))630,710,630
630 JROW=INDEX(L,1)
640 JCOLUM=INDEX(L,2)
650 DO 705 K=1,N
660 SWAP=A(K,JROW)
670 A(K,JROW)=A(K,JCOLUM)
700 A(K,JCOLUM)=SWAP
705 CONTINUE
710 CONTINUE
740 RETURN
    END

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MATI 103
MATI 104
MATI 105
MATI 106
MATI 107
MATI 108
MATI 109
MATI 110
MATI 111
MATI 112
MATI 113
MATI 114
MATI 115
MATI 116
MATI 117
MATI 118
MATI 119
MATI 120
MATI 121
MATI 122
MATI 123
MATI 124
MATI 125

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# ABLATINI ANALYSIS NOMENCLATURE

## MAIN

AA(I,J): Formula number. Gives the gram atoms of element J in species I.

AI...GI: These are the seven empirical constants for the high temperature fit (1000°K-6000°K) for the free energy functions. The first five constants (AI through EI) are used in the heat capacity fit.

AII...GII: These are the seven empirical constants for the low temperature fit (300°K-1000°K) for the free energy function.

All...A66: These are the six empirical constants for the enthalpy fit of the constituent elements (300°K-1000°K).

ALPHA: Viscous coefficient in Darcy's equation ( $\text{FT}^{-1}$ ).

AVGFW: Average molecular weight of the gas mixture.

BETA: Inertial coefficient in Darcy's equation ( $1/\text{FT}^2$ ).

CDO: Thermal conductivity of the char ( $\text{BTU}/\text{FT}\cdot\text{sec}\cdot^{\circ}\text{F}$ ).

CDOV: Thermal conductivity of the virgin material, ( $\text{BTUft}/\text{sec}\cdot^{\circ}\text{F}$ ).

CPB1: Total rate of heat absorbed by the gases in the char zone ( $\text{BTU}/\text{ft}^2\cdot\text{sec}$ ).

CPB2: Total rate of heat absorbed by the solids in the char zone ( $\text{BTU}/\text{ft}^2\cdot\text{sec}$ ).

CPS: Heat capacity of the char ( $\text{BTU}/\text{lb}\cdot^{\circ}\text{F}$ ).

CPV: Heat capacity of the virgin material (BTU/lb-°F).

DCDO: Rate of change of the thermal conductivity of the char with temperature (BTU/ft-sec-°F<sup>2</sup>).

DCDOV: Rate of change of the thermal conductivity of the virgin material with temperature (BTU/ft-sec-°F<sup>2</sup>).

DELTF: Differential change in temperature in °F for an increment of distance H.

DELTK: Differential change in temperature in °K for an increment of distance H.

DELTP: Pressure drop across the char (lbs/ft<sup>2</sup>).

DELZ: Increment of distance (in feet).

DISTAN: Char thickness in feet.

DT: Temperature gradient (°F/ft).

DTC: Temperature gradient in the char (°F/ft).

DTCC: Temperature gradient in double precision arithmetic in the char (°F/ft).

DTCI: Temperature gradient in the virgin material (°F/ft).

EK: Potential parameter /Boltzman constant.

EMIS: Char emissivity.

EPS: Porosity of the char (ft<sup>2</sup>voids/ft<sup>2</sup> total).

FW(I): Molecular weight of species I.

GASCP: Is the heat capacity of the gas mixture in (BTU/lb-°F).

GROUP: This is the bracketted term of Equation (3-36) (1/ft).

H: Runge-Kutta step size (in feet).

H11: Runge-Kutta step size in double precision arithmetic (in feet).

HCHAR: Percent of total heat absorbed in the char zone.

HDECOM: Percent of total heat absorbed in the decomposition zone.

HGAS: Percent of heat absorbed by the gas in the char zone.

HI: Initial value of Runge-Kutta step (in feet).

HREACT: Percent of heat absorbed by the reactions in the char zone.

HSOLID: Percent of heat absorbed in the solids in the char zone.

ICODE(I): Is a code to identify whether a species is a gas, or a solid. If ICODE is zero, the species is a gas. If ICODE is one, the species is a solid.

IMAX: Number of data points for EK.

ITEMP: Total number of temperature points stored in temperature profile.

JCODE(J): Is a code used to determine whether the reference state of the constituent element J is in the gas or in the solid state.

JS: Total number of slices in which the char is divided for the solution of the momentum equation.

K1: Is a counter for the number of temperature points stored during the solution of the energy equation.

MM: Is the number of elements.

NC: Number of gas species read in.

NDAT A: Number of collision integral points tabulated versus XTKE.

NN: Number of gas species in the system.

NN5: Is the total number of variables stored in Table (I,J).

NNS: Is the number of solid species in the system.

NQ: Is the total number of gas and solid species in the system.

NS: Is the total number of gas and solid species read in.

OMGA: Interpolated value of XTKE.

P: Pressure in lbs/ft<sup>2</sup>.

PL: Pressure at the front surface of the char (lbs/ft<sup>2</sup>).

Q: Is the rate of heat absorbed in the decomposition zone in (BTU/ft<sup>3</sup>-sec).

Q2: It equals  $Q/DTC$  (BTU/ft<sup>2</sup>-sec-°F).

QA: Aerodynamic heating rate (BTU/ft<sup>2</sup>-sec). Equals  $QL+QR$ .

QCZ: Heat flux in the char zone (BTU/ft<sup>2</sup>-sec).

QCZI: Heat flux in the decomposition zone (BTU/ft<sup>2</sup>-sec).

QL: Is the total heat flux at the surface (BTU/ft<sup>2</sup>-sec).

QR: Is the rate of re-radiation from the surface of the char (BTU/ft<sup>2</sup>-sec).

REAC1: Is the total rate of heat absorbed by the chemical reactions (BTU/ft<sup>2</sup>-sec).

REAC2: Heat absorbed by the chemical reactions (BTU/ft<sup>2</sup>-sec).



REACT: Equals REAC2/DTC (BTU/ft<sup>2</sup>-sec-°F).

RHO: Bulk density of the virgin material (lbs/ft<sup>3</sup>).

ROCHAR: Bulk density of the char material (lbs/ft<sup>3</sup>).

RR: Gas constant: 1.98726 (BTU/lb-mole°R).

S1...S6: These are six empirical constants for the enthalpy fit of the constituent elements (1000°K-6000°K).

SIG: Collision diameter (Angstroms).

SIGMA: Stephan-Boltzman constant ( $4.81 \times 10^{-13}$  BTU/ft<sup>2</sup>-sec-°F<sup>4</sup>).

T1(K1): Variable in which the temperature profile is stored versus distance Z. K1 is a counter.

TC: Temperature in °F.

TCHAR: Temperature at which all the virgin material has degraded to gas and char. (°K).

TFMAX: Maximum specified temperature of the front surface of the char (°F).

THICK: Is the thickness of the char zone, in inches.

THICK1: Is the thickness of the decomposition zone in inches.

TK: Interpolated value of the temperature (in °K) at a distance Z in the char.

TL: Front surface temperature of the char (°F) when the temperature profile has been defined.

TLOW(I): Maximum temperature of low temperature fit for species I. (°K).

TO: Initial temperature (°F) at Z=0.

TPREV: Temperature (°F) at the previous step.

TTTT: This is the temperature ( $^{\circ}\text{F}$ ) in double precision arithmetic. A provision has been made in the program that if the step size is less than  $8. \times 10^{-9}$  ft., the Runge-Kutta analysis is calculated in double precision arithmetic to reduce round-off error.

TVAR: Temperature in  $^{\circ}\text{K}$ .

TVIS: Interpolated value of the temperature profile ( $^{\circ}\text{F}$ ) at a distance  $Z$  along the char.

VISCOS: Viscosity of the gas (in centipoise).

VR: Surface recession velocity (ft/sec).

W: Mass flux based on the total area ( $\text{lbs}/\text{ft}^2\text{-sec}$ ).

WI: Mass flux of the gases entering the char based on the total area ( $\text{lbs}/\text{ft}^2\text{-sec}$ ).

XTKE: Product of the temperature in  $^{\circ}\text{K}$  and  $1/\text{EK}$ .

YCOMP(I,J): Array to store the concentration profile.

Y(I): Mole fraction of species  $I$ .

YI(I): Initial mole fraction of species  $I$ .

Z: Distance along the decomposition zone or the char zone (ft).

ZINC: Increment of distance at which the temperature profile is stored (ft).

ZMAX: Maximum allowable thickness of the char zone.  
(Usually 0.25 inches).

ZZ: Distance of  $Z$  in double precision arithmetic (ft).

#### INDPTH

This subroutine calculates the physical properties of

the virgin material and the pyrolysis gases.

A...E: These are five empirical constants for the heat capacity of the virgin material.

TELTKK: Increment of temperature ( $^{\circ}\text{K}$ ).

### PHMCR

This subroutine computes the heat absorbed by the decomposition of the phenolic resin and phenolic microballoons.

AREA: This is the area generated by a plot of calories versus temperature ( $^{\circ}\text{K}$ ) by the decomposition of phenolic resin during a differential thermal analysis (1350 cal/ $^{\circ}\text{K}$ ).

AREAl: This is the area generated by a plot of calories versus temperature ( $^{\circ}\text{K}$ ) by the decomposition of phenolic microballoons during a differential thermal analysis (1464 cal/ $^{\circ}\text{K}$ ).

A(I)...E(I): These are five empirical constants used to fit a curve through a portion of the plot of calories versus temperature for the phenolic microballoons.

DT: Is the temperature difference in  $^{\circ}\text{K}$  from a base temperature of  $350^{\circ}\text{C}$  ( $623^{\circ}\text{K}$ ). Below  $350^{\circ}\text{C}$ , decomposition of the virgin material has not been initiated.

DELT: Is the temperature increment ( $^{\circ}\text{K}$ ) for an increment of the Runge-Kutta Step.

H: Is the height (in calories) for the plot of calories versus temperature ( $^{\circ}\text{K}$ ).

K6: Is a code used to bypass the read statements. When K6 is one, the data is read in. When K6 is two, the read

statements are bypassed.

NUMBER: Is the number of fits used for the plots of calories versus temperature.

QMICRO: Heat absorbed by the decomposition of the phenolic microballoons (calories/gram).

QPHNLC: Heat absorbed by the decomposition of the phenolic resin (calories/gram).

#### NYLON:

This subroutine calculates the heat absorbed by the decomposition of nylon.

AREA: This is the area generated by a plot of calories versus temperature ( $^{\circ}\text{K}$ ) for the decomposition of nylon (1122 calories /  $^{\circ}\text{K}$ ) during a differential thermal analysis.

QNYLON: Heat absorbed by the decomposition of nylon (calories/gram).

#### DENSITY:

This subroutine calculates the density change of phenolic nylon and the mass flux of the pyrolysis gas.

A(J): Frequency factor of reaction J ( $\text{sec}^{-1}$ ).

COMPST: Is an integer variable giving the number of composite in the ablator. In the case of phenolic nylon, it is three.

DEFLX(I): Is the change in mass flux of composite I due to degradation ( $\text{lbs/ft}^2\text{-sec}$ ).

DRHO: Differential change in density due to degradation.

This variable is used as a criteria for stability while the solution is marching through the decomposition zone (lbs/ft<sup>3</sup>).

DRHODT(I): Rate of gas generation by the degradation of composite I (lbs/ft<sup>3</sup>-sec).

E(J): Energy of activation of reaction J used to describe the degradation of the composite (Joules/gram-mole).

MASFLX(I): Rate of change of mass flux due to the degradation of composite I (lbs/ft<sup>2</sup>-sec).

MASFRC(I): Mass fraction of each composite in the mixture of virgin material.

NREACT: Number of pseudo-order kinetic reactions used to describe the decomposition of the virgin material composite.

RATER(J): Is specific reaction velocity of reaction J (lbs/ft<sup>3</sup>-sec).

RHO: Bulk density of the composite (lbs/ft<sup>3</sup>).

RHOC(I): Residual density of composite I (lbs/ft<sup>3</sup>).

RHOCC(I): Lowest value of residual density of composite I (lbs/ft<sup>3</sup>).

RHOI(I): Initial density of composite I (lbs/ft<sup>3</sup>).

RHOII: Initial density of the virgin composite (lbs/ft<sup>3</sup>).

RHOT(I): Density of composite I at temperature T (lbs/ft<sup>3</sup>).

VOLFRC(I): Volume fraction of each composite I.

CHARPR:

This subroutine calculates the effective thermal conductivity and the heat capacity of the char.

T: Temperature in  $^{\circ}\text{R}$ .

INTRPL:

This program performs Lagrangian interpolation with non-equal step size between points.

F: Dependent variable array.

IMAX: Number of points in array.

SOM: Value of the interpolated dependent variable.

VAR: Value of X for which corresponding value of F is derived by interpolation.

X: Independent variable array.

THERM1:

This subroutine calculates the heat of formation of each chemical specie, the heat capacity of the mixture and the heat absorbed by the chemical reactions.

CPDT1: Is the sensible enthalpy gain by the constituent elements from a reference temperature of  $298.16^{\circ}\text{K}$  (calories/gram-mole).

CPMX: Heat capacity of the gas mixture (calories/gram-mole  $^{\circ}\text{K}$ ).

ENT1(I): Enthalpy of species I (calories/gram-mole).

ENT(I): Heat of formation of species I (calories/gram-mole).

HEAT1: Rate of heat generated, or absorbed, by the chemical reactions (calories/cm<sup>3</sup>-sec).

KINET:

This program computes the rate of reaction of each chemical species.

AEF(J): Activation energy of reaction J (calories/gram-mole).

AF(J): Frequency factor of reaction J (sec<sup>-1</sup>).

DELZZ: Runge-Kutta step size (cm.).

DLFLUX(I): Differential change in molal flux due to the chemical reaction of species I. This variable is used for the purpose of controlling the step size (gram-mole/cm<sup>2</sup>-sec).

FLUXMO(I): Molal flux of each chemical species I (gram-moles/cm<sup>2</sup>-sec).

HEAT: Rate of heat generated or absorbed by the chemical reactions (BTU/ft<sup>3</sup>-sec).

K2: Is a counter to keep track of the number of temperature points stored in Table (I,J).

K7: When K7 is one, initialization occurs and subroutine INOUT is called. When it is 2, this is bypassed.

KOS: Total number of variables stored in the Table (I,J) array.

KSP: Number of gas components in the chemical system.

KSP1: Number of gas and solid species in the chemical system.

NPEX(I,J): Power on the concentration of product I in

reaction J.

P: Pressure of the system in atmosphere.

PERCE(J): Mole percent of species J.

PSC(I,J): Stoichiometric coefficient of the product I in reaction J.

R: Gas constant ( $82.06 \text{ cm}^3\text{-atm/gram-mole } ^\circ\text{K}$ ).

RATE(J): Rate of formation of species I ( $\text{gram-moles/cm}^3\text{-sec}$ ).

RATER(J): Specific reaction velocity of reaction J ( $\text{gram-moles/cm}^3\text{-sec}$ ).

RK(J): Reverse reaction rate constant of reaction J.

RR: Gas constant ( $1.98726 \text{ calories/gram-mole } ^\circ\text{K}$ ).

SF(J): Power on the temperature of the Arrhenius type kinetic expression.

SPCIE1(J): Specie identification name.

T: Temperature ( $^\circ\text{K}$ ).

TABLE(I,J): Is an array where I represents the number of variables stored and J the number of temperature points. The variables stored are in the following order: T, HEAT, WNEW, AVGFW AND KSPl values of Y1(I).

TESS: Is the absolute maximum value of DLFLUX(I). This variable is used in controlling the step size for stability.

TF: Temperature ( $^\circ\text{F}$ ).

TPREV: Is the previous value of the temperature ( $^\circ\text{K}$ ).

WNEW: Total mass flux of the gases ( $\text{lbs/ft}^2\text{-sec}$ ).

XMW (I): Molecular weight of species I.

Y1(I): Mole fraction of species I.



INPUT:

This subroutine reads in the kinetic data.

AK(J): Empirical constant for the fit of the equilibrium constant with temperature.

BK(J): Empirical constant for the fit of the equilibrium constant with temperature.

EKMAX(J): Maximum allowable value for the equilibrium constant of reaction J.

EKMIN(J): Minimum allowable value for the equilibrium constant of reaction J.

NCOEF(J): Is the sum of the stoichiometric coefficient of the products minus the reactants.

INPUT FORMAT: A Typical Input for Equilibrium Flow.\*

<u>CARD-1:</u>	FORMAT (5I6)	<u>COLUMNS:</u>
NC = 19		1-6
NNS = 1		7-12
MM = 4		13-18
KODE = 1		19-24
KEY = 2		25-30

<u>CARD-2:</u>	FORMAT (F10.3, 10X, 4F10.3)	
PL = 2160.		1-10
TO = 500		21-30
EPS = .8		31-40
ZL = .35		41-50
HI = .000007		51-60

<u>CARD-3:</u>	FORMAT(3E15.5, F15.5)	
ALPHA = .5E9		1-15
BETA = .5E5		16-30
SIGMA = .48E-12		31-45
EMIS = .90		46-60

<u>CARD-4</u>	FORMAT (3E10.3)	
DTC = 3000.		1-10
TCHAR = 1073.		11-20
VT = 1.E-3		21-30

---

\*See Table B-2 for the complete input data set.

<u>CARD-5</u>	FORMAT (6E10.3, I3)	<u>COLUMNS</u>
S1(1)	= 1.363250E0	1-10
S2(1)	= 1.85605E-3	11-20
S3(1)	= -7.6675E-7	21-30
S4(1)	= .151043E-9	31-40
S5(1)	= -1.139E-14	41-50
S6(1)	= -6.46972E2	51-60
JCODE(1)	= 1	61-63

<u>CARD-6</u>	FORMAT (6E10.3)	
A11(1)	= -.712442E0	1-10
A22(1)	= 7.34065E-3	11-20
A33(1)	= -5.5262E-6	21-30
A44(1)	= 1.51400E-9	31-40
A55(1)	= -2.382E-14	41-50
A66(1)	= -6.80533E1	51-60

CARD-5 and CARD-6 are read sequentially MM times as is specified in CARD-1. For this particular example MM = 4.

<u>CARD-7</u>	FORMAT (10X, 3E10.3, 2X, 2A3, I4)	
TLOW (1)	= 1000.	11-20
FW(1)	= 1.008	21-30
YI(1)	= .739503E-7	31-40
SPCIE 1(1)	=	43-45
SPCIE 2 (1)	= H	46-48
ICODE(1)	= 0	49-52

CARD-8      FORMAT (7E10.3)      COLUMNS

AI(1) = 2.500000E0	1-10
BI(1) = 0.	11-20
CI(1) = 0.	21-30
DI(1) = 0.	31-40
EI(1) = 0.	41-50
FI(1) = 2.547050E4	51-60
GI(1) = -4.6001E-1	61-70

CARD-9      FORMAT (7E10.3)

AII(1) = 2.500000E0	1-10
BII(1) = 0.	11-20
CII(1) = 0.	21-30
DII(1) = 0.	31-40
EII(1) = 0.	41-50
FII(1) = 2.547050E-4	51-60
GII(1) = 4.6001E-1	61-70

CARD-10      FORMAT (4E10.3)

AA(1,1) = 0.	1-10
AA(1,2) = 1.	11-20
AA(1,3) = 0.	21-30
AA(1,4) = 0.	31-40

CARD-7, CARD-8, CARD-9 and CARD-10 are read in sequentially as a group, (NC+NNS) number of times. Only the data for Specie 1, in this case hydrogen atoms, is presented.

## COLUMNS

CARD-11 FORMAT (2F15.5)

EK(1) = 33.3 1-15

SIG(1) = 2.986 16-30

CARD-11 is read NC number of times as specified by  
CARD-1.

CARD-12      FORMAT (I6)

NDA = 34 i-6

CARD-13      FORMAT (2F15.5)

XTKE(1) = 0.30 1-15

ZOMGA(1) = 2.785 16-30

CARD-13 is repeated NDATA number of times as specified by CARD-12.

CARDS-1 through 13 are read in the MAIN program. These cards define the physical conditions of the system. In addition they provide the thermodynamic data and the physical constants for the pyrolysis species. CARDS-14 through 19 provide the thermophysical information for the virgin material and also the kinetic data for the degradation of the polymer.

CARD-14 FORMAT (5E12.6)

A = 0.37000070E0 1-12

B = 0.7367133E-4 13-24

C = 0.1532518E-5 25-36

D = -.1962704E-8 37-48

E = .8857809E-12 49-60

CARD-14 is read in subroutine INDPATH.

<u>CARD-15</u>	FORMAT (5E12.8)	<u>COLUMNS</u>
A(1) = 0.10561790E0		1-12
B(1) = -1.836062E-2		13-24
C(1) = 1.7580490E-3		25-36
D(1) = -1.678598E-5		37-48
E(1) = 4.7310570E-8		49-60

<u>CARD-16</u>	FORMAT (5E12.8)	
A1(1) = -.35642660E-1		1-12
B1(1) = 4.5790730E-2		13-24
C1(1) = 1.2298170E-4		25-36
D1(1) = -.8277667E-7		37-48
E1(1) = -.2279748E-7		49-60

CARD-15 and CARD-16 are read sequentially four times in subroutine PHMCR. For a thorough explanation on the sources of data for the phenolic resin see Appendix C.

<u>CARD-17</u>	FORMAT (2I6)	
COMPST = 3		1-6
NREACT = 7		6-12

Card-17 is read in subroutine DENSITY as well as CARDS 18 and 19.

<u>CARD-18</u>	FORMAT (4X, I6, 3E10.8)	
I = 1		5-10
A(1) = 8.3000E14		11-20
E(1) = 232.0		21-30

COLUMNS

XN(I,1) = 1.0

31-40

CARD-18 is read NREACT number of times and the index in I changes from 1 through 3 depending on whether the data is for nylon or for phenolic or for the microballoons.

CARD-19      FORMAT (3E10.3)

RHOI(1) = 68.6      1-10

RHOC(1) = 5.145      11-21

MASFR(1) = 0.4      21-30

CARD-19 is repeated COMPST number of times.

CARD-20      FORMAT (I1)

IPRINT = 1

CARD-20 is read in subroutine CHEMEQ.

**TABLE B-2. Typical Input Data for Equilibrium Analysis**

19	1	4	1	2																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					</
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3.5023E00 1.159E-02-4.4745E-6 7.945E-10-5.323E-14 4.5439E03 2.4667E00	DATA	35
1.120244E0 1.3906E-2 2.6568E-6-1.1560E-85.2387E-125.332889E3 1.58378E1	DATA	36
2.00000E0 4.00000E0 0.00000E0 0.00000E0	DATA	37
1000.E0 30.070E0.208273E-5 C2H6 0	DATA	38
.1430799E1.188898E-1-.70440E-5.118720E-8-.7445E-13-.114311E5.1401321E2	DATA	39
.2882039E1.103219E-1.119142E-4-.14832E-7.44749E-11-.116209E5.7597900E1	DATA	40
2.00000E0 6.00000E0 0.00000E0 0.00000E0	DATA	41
1000.E0 28.016E0 0.1880617 N2 0	DATA	42
2.854576E0 1.5976E-3-6.2566E-71.1316E-10-7.69E-15-8.90174E2 6.39029E0	DATA	43
3.691615E0-1.3333E-32.65031E-6-9.769E-10-9.977E-14-1.06283E3 2.28750E0	DATA	44
0.000000E0 0.00000E0 2.00000E0 0.00000E0	DATA	45
1000.E0 17.032E0.261467E-3 NH3 0	DATA	46
2.149399E06.49285E-3-2.2695E-63.7394E-10-2.361E-14-6.40196E3 9.23891E0	DATA	47
3.77162E00-4.8621E-49.8742E-06-9.5679E-93.1313E-12-6.72810E3 1.4654E00	DATA	48
0.00000E00 3.00000E0 1.00000E0 0.00000E0	DATA	49
1000.E0 27.027E0.206307E-4 HCN 0	DATA	50
3.653803E03.44363E-3-1.2585E-62.1692E-10-1.430E-141.442180E42.372602E0	DATA	51
2.168115E01.07290E-2-1.5088E-51.19330E-8-3.700E-121.468290E49.281020E0	DATA	52
1.000000E0 1.00000E0 1.00000E0 0.00000E0	DATA	53
1000.E0 18.016E0 0.1063185 H2O 0	DATA	54
2.67075E0 3.0317E-3 -8.535E-7 1.179E-10-6.197E-15-2.9889E04 6.88383E0	DATA	55
4.15650E00-1.7244E-35.6982E-06-4.5930E-91.4234E-12-3.02888E4-6.8616E-1	DATA	56
0.000000E0 2.00000E0 0.00000E0 1.00000E0	DATA	57
1000.E0 17.008E0 1.0000E-9 OH 0	DATA	58
2.889554E09.98350E-4-2.1880E-71.9803E-11-3.845E-163.881179E35.559701E0	DATA	59
3.823470E0-1.1187E-31.24668E-6-2.103E-10-5.254E-143.585278E35.8253E-01	DATA	60
0.000000E0 1.00000E0 0.00000E0 1.00000E0	DATA	61
1000.E0 44.011E0 .02711201 CO2 0	DATA	62
4.4129E003.1923E-03 -1.298E-6 2.415E-10-1.674E-14-4.8944E04-7.2876E-1	DATA	63
2.170100E0 1.0378E-2-1.0734E-56.34592E-9-1.628E-12-4.83526E4 1.06644E1	DATA	64
1.00000E0 0.00000E0 0.00000E0 2.00000E0	DATA	65
1000.E0 28.011E0 0.1077713 CO 0	DATA	66
2.9512E00 1.5526E-3-6.1911E-7 1.135E-10-7.788E-15-1.4232E04 6.5314E00	DATA	67
3.787133E0-2.171E-035.07573E-6-3.4738E-97.7217E-13-1.43635E4 2.63355E0	DATA	68

1.00000E0 0.00000E0 0.00000E0 1.00000E0	DATA	69
1000.F0 26.019E0 1.0000E-9 CN 0	DATA	70
3.602263E03.40862F-49.71624E-8-1.582F-11-4.142E-164.731037E43.552052E0	DATA	71
3.852814E0-2.7632E-36.85704E-6-5.413E-091.4906E-124.740969E42.971802E0	DATA	72
1.000000E0 0.00000E0 1.00000E0 0.00000E0	DATA	73
1000.E0 25.030E0 1.0000E-9 C2H 0	DATA	74
.3513479E1.358906E-2-.13231E-5.230520E-9-.1530E-13.5788759E5.4523285E1	DATA	75
.3006269E1.553788E-2-.35112E-5.124860E-8-.1896E-12.5796960E5.6920349E1	DATA	76
2.000000E0 1.00000E0 0.00000E0 0.00000E0	DATA	77
1000.E0 37.041E0 1.0000E-9 C3H 0	DATA	78
.3964709E1.620030E-2-.22655E-5.371712E-9-.2262E-13.6283285E5.3467072E1	DATA	79
.2473840E1.117509E-1-.80448E-5.272896E-8-.3544E-12.6307721E5.1054254E2	DATA	80
3.000000E0 1.00000E0 0.00000E0 0.00000E0	DATA	81
1000.E0 39.052E0 1.0000E-9 C4H 0	DATA	82
.5873679E1.740338E-2-.27289E-5.443720E-9-.2637E-13.7605163E5-.401004E1	DATA	83
.2695820E1.226768E-1-.24508E-4.131474E-7-.2673E-11.7648881E5.1039807E2	DATA	84
4.000000E0 1.00000E0 0.00000E0 0.00000E0	DATA	85
1000.E0 36.033E0 1.0000E-9 C3 0	DATA	86
4.712474E02.90265F-3-1.2142E-62.2847E-10-1.599E-149.375270E4-2.53044E0	DATA	87
2.632587E09.41857E-3-9.5932E-65.57955E-9-1.424E-129.431148E48.078826E0	DATA	88
3.000000E0 0.00000E0 0.00000E0 0.00000E0	DATA	89
1000.E0 12.011E0 7.125731 C 1	DATA	90
1.36325E001.85605E-3-7.6675E-71.5104E-10-1.139E-14-6.4967E02-7.9890E00	DATA	91
-7.1244E-17.34065E-3-5.5262E-6 1.514E-09-2.382E-14-6.80533E1 2.79326E0	DATA	92
1.0000E00 0.00000E0 0.0000E00 0.0000E00	DATA	93
33.3 2.986 H	DATA	94
33.3 2.986 H2	DATA	95
136.5 3.822 CH3	DATA	96
136.5 3.822 CH4	DATA	97
185.0 4.221 C2H2	DATA	98
205.0 4.232 C2H4	DATA	99
230.0 4.418 C2H6	DATA	100
91.5 3.681 N2	DATA	101
356.0 2.649 H2O	DATA	102

335.	4.31	HCN
312.0	3.432	NH3
113.0	3.433	OH
190.0	3.996	CO2
110.0	3.590	CO
335.	4.31	CN
185.0	4.221	C2H
185.0	4.221	C3H
185.0	4.221	C4H
185.0	4.221	C3

34	
0.30	2.785
0.35	2.628
0.40	2.492
0.45	2.368
0.50	2.257
0.55	2.156
0.60	2.065
0.65	1.982
0.70	1.908
0.75	1.841
0.80	1.780
0.85	1.725
0.90	1.675
0.95	1.629
1.00	1.587
1.10	1.514
1.20	1.452
1.30	1.399
1.50	1.314
1.70	1.248
1.90	1.197
2.2	1.138
2.6	1.081

DATA 103
DATA 104
DATA 105
DATA 106
DATA 107
DATA 108
DATA 109
DATA 110
DATA 111
DATA 112
DATA 113
DATA 114
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DATA 123
DATA 124
DATA 125
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DATA 133
DATA 134
DATA 135
DATA 136

3.2	1.022	DATA 137
200.0	0.5320	DATA 138
400.0	0.4811	DATA 139
0.3700070E0	0.7367133E-4 .1532518E-5-.1962704E-8.8857809E-12	DATA 140
0.1056179E0	-1.836062E-2 1.758049E-3-1.678598E-5 4.731057E-8	DATA 141
-.3564266E-1	4.579073E-2 1.229817E-4-.8277667E-7-.2279748E-7	DATA 142
173.99268E0	-4.816270E0 .50990242E-1-2.383797E-4 4.135187E-7	DATA 143
-50.09959E0	1.707140E0 -.1945725E-1 .9382376E-4-.1648646E-6	DATA 144
52.578338E0	-.8655753E0 .51867970E-2-.1242327E-4 .1021600E-7	DATA 145
-169.8485E0	3.907641E0 -.3215650E-1 .1127232E-3-.1410145E-6	DATA 146
7.0	0.8727	DATA 147
10.0	0.8242	DATA 148
20.0	0.7432	DATA 149
40.0	0.6718	DATA 150
70.0	0.6194	DATA 151
100.0	0.5882	DATA 152
4.0	0.9700	DATA 153
5.0	0.9269	DATA 154
-1731.992E0	20.881448E0 -.9146933E-1 .1739896E-3-.1218719E-6	DATA 155
3	7	DATA 156
1	8.3000E14 232.000E0 1.00000E0	DATA 157
2	5.10000E8 114.000E0 3.00000E0	DATA 158
2	2.50000E5 100.000E0 1.30000E0	DATA 159
2	2.00000E7 140.000E0 3.10000E0	DATA 160
3	2.00000E5 70.000E0 2.00000E0	DATA 161
3	9.70000E6 122.000E0 2.00000E0	DATA 162
3	1.3000E10 172.000E0 3.00000E0	DATA 163
68.6000E0	5.14500E0 0.4000E0	DATA 164
80.0000E0	43.2800E0 0.2500E0	DATA 165
17.8000E0	9.64760E0 0.3500E0	DATA 166
1		DATA 167
-855.3400E0	10.103099E0 -.4343457E-1 .8122788E-4-.5603327E-7	DATA 168

TABLE B-3. Typical Output for Equilibrium Analysis

INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

THEORETICAL

CHAR BACK TEMPERATURE (OF)= 1524.8	NUMBER OF GAS COMPONENTS= 19
INITIAL SLOPE(OF/FT)= 3000.0	INITIAL DENSITY OF COMPOSITE(LBS/FT**3)= 34.94
THICKNESS OF CHAR(INCHES)=0.022392	THICKNESS OF DECOMPOSITION ZONE=0.053250
TOTAL MASS FLUX(LBS/FT2-SEC)=.034942	GAS MASS FLUX AT THE SURFACE= .074805
FRONT SURFACE TEMPERATURE(OF)=5500.0	SURFACE RECESSION VELOCITY(FT/SEC)=0.00100
RATE OF HEAT ABSORBED IN THE CHAR ZONE(BTU/FT**2-SEC)=16872.277	
RATE OF HEAT ABSORBED IN THE DECOMPOSITION ZONE(BTU/FT2-SEC=) 20.638	
PERCENT OF TOTAL HEAT ABSORBED IN THE CHAR ZONE= 0.9987781E 02	
PERCENT OF TOTAL HEAT ABSORBED IN DECOMP-ZONE= 0.1221668E 00	
PERCENT OF HEAT ABSORBED BY THE GAS IN THE CHAR ZONE= 0.4576713E 00	
PERCENT OF HEAT ABSORBED BY THE SOLIDS IN THE CHAR ZONE= 0.8026010E-01	
PERCENT OF HEAT ABSORBED BY REACTION IN THE CHAR ZONE= 0.9946208E 02	

# INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

TEMPERATURE DROP (OF) = 3981.0

PRESSURE DROP (LB/FT2) = 9.6

SURFACE HEAT FLUX (BTU/FT2-SEC) = 16892.92

RADIANT HEAT FLUX BTU/FT2-SEC)=, 547.71

AERODYNAMIC HEAT FLUX(BTU/FT2-SEC)= 17440.63

CHAR DEPTH (FT)	0.0044	0.0045	0.0045	0.0046	0.0046
TEMPERATURE (OF)	1524.8	1533.0	1542.2	1552.3	1563.3
PRESSURE (LB/FT2)	2169.6	2169.5	2169.4	2169.3	2169.2
MASS FLUX(LB/FT2-SEC)	0.0216	0.0266	0.0266	0.0265	0.0264

GAS COMPONENT		COMPOSITION (MOLE/MOLE GAS)				
1	H	0.7395E-07	0.2825E-07	0.3112E-07	0.3528E-07	0.4074E-07
2	H2	0.4578E 01	0.8869E 00	0.8880E 00	0.8894E 00	0.8908E 00
3	CH3	0.1038E-06	0.3446E-07	0.3658E-07	0.3952E-07	0.4299E-07
4	CH4	0.1605E 00	0.2709E-01	0.2605E-01	0.2476E-01	0.2355E-01
5	C2H2	0.3903E-07	0.1627E-07	0.1794E-07	0.2036E-07	0.2353E-07
6	C2H4	0.2864E-05	0.7532E-06	0.7683E-06	0.7881E-06	0.8090E-06
7	C2H6	0.2083E-05	0.3445E-06	0.3289E-06	0.3097E-06	0.2919E-06
8	N2	0.1881E 00	0.3549E-01	0.3545E-01	0.3539E-01	0.3534E-01
9	NH3	0.2615E-03	0.4901E-04	0.4783E-04	0.4634E-04	0.4489E-04
10	HCN	0.2063E-04	0.7020E-05	0.7429E-05	0.7995E-05	0.8661E-05
11	H2O	0.1063E 00	0.3443E-02	0.3247E-02	0.3010E-02	0.2797E-02
12	OH	0.1000E-08	0.5333E-12	0.5719E-12	0.6259E-12	0.6912E-12
13	CO2	0.2711E-01	0.1753E-03	0.1630E-03	0.1484E-03	0.1356E-03
14	CO	0.1078E 00	0.4684E-01	0.4700E-01	0.4719E-01	0.4736E-01
15	CN	0.1000E-08	0.3660E-14	0.4324E-14	0.5360E-14	0.7033E-14
16	C2H	0.1000E-08	0.6916E-16	0.8449E-16	0.1091E-15	0.1533E-15
17	C3H	0.1000E-08	0.2759E-17	0.3422E-17	0.4499E-17	0.6540E-17
18	C4H	0.1000E-08	0.3247E-21	0.4201E-21	0.5797E-21	0.9319E-21
19	C3	0.1000E-08	0.6734E-27	0.9151E-27	0.1329E-26	0.2437E-26
20	C	0.7126E 01	0.1326E 01	0.1326E 01	0.1325E 01	0.1324E 01

# INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0047	0.0047	0.0048	0.0048	0.0049
TEMPERATURE (OF)	1575.3	1588.3	1599.4	1614.9	1632.2
PRESSURE (LB/FT2)	2169.1	2169.0	2168.9	2168.8	2168.6
MASS FLUX(LB/FT2-SEC)	0.0264	0.0263	0.0263	0.0262	0.0261

## GAS COMPONENT

## COMPOSITION (MOLE/MOLE GAS)

1	H	0.4693E-07	0.5412E-07	0.6186E-07	0.7411E-07	0.9005E-07
2	H2	0.8921E 00	0.8935E 00	0.8946E 00	0.8960E 00	0.8975E 00
3	CH3	0.4682E-07	0.5109E-07	0.5529E-07	0.6153E-07	0.6912E-07
4	CH4	0.2231E-01	0.2103E-01	0.2003E-01	0.1873E-01	0.1737E-01
5	C2H2	0.2713E-07	0.3131E-07	0.3580E-07	0.4293E-07	0.5220E-07
6	C2H4	0.8312E-06	0.8552E-06	0.8765E-06	0.9060E-06	0.9395E-06
7	C2H6	0.2738E-06	0.2552E-06	0.2409E-06	0.2225E-06	0.2034E-06
8	N2	0.3529E-01	0.3524E-01	0.3520E-01	0.3515E-01	0.3510E-01
9	NH3	0.4340E-04	0.4183E-04	0.4057E-04	0.3890E-04	0.3710E-04
10	HCN	0.9392E-05	0.1021E-04	0.1101E-04	0.1219E-04	0.1363E-04
11	H2O	0.2581E-02	0.2361E-02	0.2197E-02	0.1989E-02	0.1777E-02
12	OH	0.7636E-12	0.8451E-12	0.9270E-12	0.1050E-11	0.1202E-11
13	CO2	0.1228E-03	0.1099E-03	0.1006E-03	0.8893E-04	0.7733E-04
14	CO	0.4753E-01	0.4770E-01	0.4782E-01	0.4798E-01	0.4814E-01
15	CN	0.9050E-14	0.1159E-13	0.1477E-13	0.2056E-13	0.2916E-13
16	C2H	0.2083E-15	0.2804E-15	0.3776E-15	0.5674E-15	0.8686E-15
17	C3H	0.9113E-17	0.1256E-16	0.1735E-16	0.2704E-16	0.4293E-16
18	C4H	0.1395E-20	0.2055E-20	0.3057E-20	0.5297E-20	0.9335E-20
19	C3	0.3976E-26	0.6346E-26	0.1033E-25	0.2042E-25	0.4091E-25
20	C	0.1323E 01	0.1322E 01	0.1321E 01	0.1320E 01	0.1319E 01

# INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0049	0.0050	0.0050	0.0051	0.0051
TEMPERATURE (OF)	1651.6	1672.9	1690.8	1718.2	1749.7
PRESSURE (LB/FT2)	2168.5	2168.4	2168.3	2168.2	2168.0
MASS FLUX(LB/FT2-SEC)	0.0260	0.0259	0.0259	0.0258	0.0257

## GAS COMPONENT

## COMPOSITION (MOLE/MOLE GAS)

1	H	0.1103E-06	0.1391E-06	0.1690E-06	0.2226E-06	0.3076E-06
2	H2	0.8990E 00	0.9005E 00	0.9016E 00	0.9032E 00	0.9048E 00
3	CH3	0.7817E-07	0.8973E-07	0.1006E-06	0.1187E-06	0.1435E-06
4	CH4	0.1597E-01	0.1460E-01	0.1357E-01	0.1212E-01	0.1070E-01
5	C2H2	0.6394E-07	0.8072E-07	0.9807E-07	0.1292E-06	0.1785E-06
6	C2H4	0.9769E-06	0.1019E-05	0.1055E-05	0.1110E-05	0.1175E-05
7	C2H6	0.1839E-06	0.1654E-06	0.1515E-06	0.1324E-06	0.1141E-06
8	N2	0.3504E-01	0.3498E-01	0.3494E-01	0.3489E-01	0.3483E-01
9	NH3	0.3521E-04	0.3329E-04	0.3179E-04	0.2964E-04	0.2741E-04
10	HCN	0.1534E-04	0.1752E-04	0.1955E-04	0.2293E-04	0.2756E-04
11	H2O	0.1564E-02	0.1369E-02	0.1227E-02	0.1035E-02	0.8588E-03
12	OH	0.1386E-11	0.1626E-11	0.1857E-11	0.2247E-11	0.2801E-11
13	CO2	0.6591E-04	0.5590E-04	0.4880E-04	0.3947E-04	0.3133E-04
14	CO	0.4830E-01	0.4843E-01	0.4853E-01	0.4866E-01	0.4877E-01
15	CN	0.4139E-13	0.6286E-13	0.8968E-13	0.1452E-12	0.2614E-12
16	C2H	0.1322E-14	0.2198E-14	0.3401E-14	0.6073E-14	0.1247E-13
17	C3H	0.6748E-16	0.1171E-15	0.1884E-15	0.3522E-15	0.7705E-15
18	C4H	0.1607E-19	0.3149E-19	0.5682E-19	0.1208E-18	0.3177E-18
19	C3	0.7836E-25	0.1777E-24	0.3704E-24	0.9182E-24	0.3032E-23
20	C	0.1318E 01	0.1317E 01	0.1317E 01	0.1316E 01	0.1315E 01



# INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0052	0.0052	0.0053	0.0053	0.0053
TEMPERATURE (OF)	1785.2	1824.9	1860.8	1913.7	1974.2
PRESSURE (LB/FT2)	2167.9	2167.8	2167.6	2167.5	2167.3
MASS FLUX(LB/FT2-SEC)	0.0256	0.0255	0.0255	0.0254	0.0253

## GAS COMPONENT

## COMPOSITION (MOLE/MOLE GAS)

1	H	0.4346E-06	0.6357E-06	0.8825E-06	0.1406E-05	0.2327E-05
2	H2	0.9063E 00	0.9077E 00	0.9087E 00	0.9100E 00	0.9112E 00
3	CH3	0.1760E-06	0.2200E-06	0.2667E-06	0.3503E-06	0.4706E-06
4	CH4	0.9310E-02	0.8021E-02	0.7032E-02	0.5831E-02	0.4746E-02
5	C2H2	0.2521E-06	0.3682E-06	0.5105E-06	0.8112E-06	0.1338E-05
6	C2H4	0.1250E-05	0.1335E-05	0.1414E-05	0.1532E-05	0.1671E-05
7	C2H6	0.9659E-07	0.8083E-07	0.6904E-07	0.5515E-07	0.4308E-07
8	N2	0.3477E-01	0.3472E-01	0.3468E-01	0.3463E-01	0.3458E-01
9	NH3	0.2514E-04	0.2291E-04	0.2110E-04	0.1878E-04	0.1652E-04
10	HCN	0.3359E-04	0.4169E-04	0.5028E-04	0.6558E-04	0.8749E-04
11	H2O	0.6975E-03	0.5585E-03	0.4588E-03	0.3470E-03	0.2552E-03
12	OH	0.3549E-11	0.4595E-11	0.5745E-11	0.7885E-11	0.1112E-10
13	CO2	0.2419E-04	0.1837E-04	0.1440E-04	0.1019E-04	0.6964E-05
14	CO	0.4887E-01	0.4895E-01	0.4901E-01	0.4906E-01	0.4910E-01
15	CN	0.4838E-12	0.9605E-12	0.1726E-11	0.3964E-11	0.9694E-11
16	C2H	0.2630E-13	0.6068E-13	0.1236E-12	0.3389E-12	0.9994E-12
17	C3H	0.1729E-14	0.4287E-14	0.9273E-14	0.2767E-13	0.8921E-13
18	C4H	0.8524E-18	0.2603E-17	0.6695E-17	0.2552E-16	0.1064E-15
19	C3	0.1011E-22	0.3991E-22	0.1269E-21	0.6517E-21	0.3708E-20
20	C	0.1314E 01	0.1313E 01	0.1313E 01	0.1312E 01	0.1312E 01

# INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0054	0.0054	0.0055	0.0055	0.0056
TEMPERATURE (OF)	2042.4	2112.4	2197.7	2292.8	2397.8
PRESSURE (LB/FT2)	2167.2	2167.0	2166.8	2166.6	2166.4
MASS FLUX(LB/FT2-SEC)	0.0253	0.0252	0.0252	0.0252	0.0251

## GAS COMPONENT

## COMPOSITION (MOLE/MOLE GAS)

1	H	0.3734E-05	0.6813E-05	0.1164E-04	0.2371E-04	0.4163E-04
2	H2	0.9121E 00	0.9130E 00	0.9136E 00	0.9142E 00	0.9145E 00
3	CH3	0.6200E-06	0.8796E-06	0.1200E-05	0.1806E-05	0.2503E-05
4	CH4	0.3916E-02	0.3064E-02	0.2465E-02	0.1851E-02	0.1460E-02
5	C2H2	0.2138E-05	0.3878E-05	0.6586E-05	0.1328E-04	0.2311E-04
6	C2H4	0.1810E-05	0.2002E-05	0.2189E-05	0.2459E-05	0.2701E-05
7	C2H6	0.3420E-07	0.2547E-07	0.1962E-07	0.1391E-07	0.1046E-07
8	N2	0.3453E-01	0.3448E-01	0.3443E-01	0.3436E-01	0.3428E-01
9	NH3	0.1466E-04	0.1258E-04	0.1099E-04	0.9188E-05	0.7927E-05
10	HCN	0.1145E-03	0.1613E-03	0.2186E-03	0.3265E-03	0.4499E-03
11	H2O	0.1917E-03	0.1332E-03	0.9657E-04	0.6331E-04	0.4454E-04
12	OH	0.1533E-10	0.2307E-10	0.3320E-10	0.5375E-10	0.7901E-10
13	CO2	0.4893E-05	0.3125E-05	0.2104E-05	0.1255E-05	0.8153E-06
14	CO	0.4913E-01	0.4914E-01	0.4915E-01	0.4915E-01	0.4915E-01
15	CN	0.2247E-10	0.6526E-10	0.1691E-09	0.6012E-09	0.1607E-08
16	C2H	0.2765E-11	0.1004E-10	0.3179E-10	0.1483E-09	0.4848E-09
17	C3H	0.2687E-12	0.1085E-11	0.3781E-11	0.2010E-10	0.7228E-10
18	C4H	0.4091E-15	0.2246E-14	0.1034E-13	0.8052E-13	0.3819E-12
19	C3	0.1921E-19	0.1529E-18	0.9847E-18	0.1226E-16	0.8116E-16
20	C	0.1311E 01	0.1311E 01	0.1310E 01	0.1310E 01	0.1310E 01

# INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0056	0.0057	0.0057	0.0058	0.0058
TEMPERATURE (OF)	2512.8	2640.8	2773.8	2915.4	3064.1
PRESSURE (LB/FT2)	2166.2	2166.0	2165.7	2165.5	2165.2
MASS FLUX(LB/FT2-SEC)	0.0251	0.0251	0.0252	0.0252	0.0253

## GAS COMPONENT

## COMPOSITION (MOLE/MOLE GAS)

1	H	0.7908E-04	0.1569E-03	0.3278E-03	0.5949E-03	0.1055E-02
2	H2	0.9148E 00	0.9148E 00	0.9145E 00	0.9140E 00	0.9131E 00
3	CH3	0.3628E-05	0.5338E-05	0.8087E-05	0.1135E-04	0.1566E-04
4	CH4	0.1113E-02	0.8550E-03	0.6388E-03	0.4988E-03	0.3961E-03
5	C2H2	0.4340E-04	0.8490E-04	0.1743E-03	0.3115E-03	0.5433E-03
6	C2H4	0.3004E-05	0.3344E-05	0.3754E-05	0.4130E-05	0.4515E-05
7	C2H6	0.7545E-08	0.5509E-08	0.3887E-08	0.2890E-08	0.2194E-08
8	N2	0.3417E-01	0.3401E-01	0.3376E-01	0.3347E-01	0.3310E-01
9	NH3	0.6694E-05	0.5663E-05	0.4706E-05	0.4021E-05	0.3464E-05
10	HCN	0.6478E-03	0.9462E-03	0.1422E-02	0.1980E-02	0.2710E-02
11	H2O	0.2981E-04	0.2034E-04	0.1329E-04	0.9246E-05	0.6610E-05
12	OH	0.1226E-09	0.1947E-09	0.3209E-09	0.4828E-09	0.7135E-09
13	CO2	0.4985E-06	0.3146E-06	0.1883E-06	0.1215E-06	0.8125E-07
14	CO	0.4915E-01	0.4914E-01	0.4914E-01	0.4913E-01	0.4911E-01
15	CN	0.4914E-08	0.1681E-07	0.6230E-07	0.1754E-06	0.4790E-06
16	C2H	0.1861E-08	0.8344E-08	0.4114E-07	0.1439E-06	0.4886E-06
17	C3H	0.3090E-09	0.1578E-08	0.8920E-08	0.3456E-07	0.1301E-06
18	C4H	0.2231E-11	0.1672E-10	0.1414E-09	0.7406E-09	0.3790E-08
19	C3	0.6891E-15	0.8254E-14	0.1142E-12	0.8607E-12	0.6402E-11
20	C	0.1309E 01	0.1309E 01	0.1308E 01	0.1307E 01	0.1305E 01

# INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0059	0.0059	0.0060	0.0060	0.0061
TEMPERATURE (OF)	3218.7	3379.1	3545.6	3719.7	3904.3
PRESSURE (LB/FT2)	2164.9	2164.5	2164.2	2163.8	2163.4
MASS FLUX(LB/FT2-SEC)	0.0254	0.0256	0.0260	0.0264	0.0270

## GAS COMPONENT

## COMPOSITION (MOLE/MOLE GAS)

1	H	0.1853E-02	0.3336E-02	0.6108E-02	0.9967E-02	0.1672E-01
2	H2	0.9115E 00	0.9087E 00	0.9039E 00	0.8974E 00	0.8865E 00
3	CH3	0.2142E-04	0.2968E-04	0.4135E-04	0.5383E-04	0.7068E-04
4	CH4	0.3164E-03	0.2489E-03	0.1938E-03	0.1575E-03	0.1253E-03
5	C2H2	0.9377E-03	0.1653E-02	0.2956E-02	0.4717E-02	0.7701E-02
6	C2H4	0.4917E-05	0.5367E-05	0.5846E-05	0.6231E-05	0.6606E-05
7	C2H6	0.1678E-08	0.1260E-08	0.9331E-09	0.7268E-09	0.5509E-09
8	N2	0.3260E-01	0.3189E-01	0.3089E-01	0.2983E-01	0.2839E-01
9	NH3	0.2989E-05	0.2545E-05	0.2142E-05	0.1848E-05	0.1560E-05
10	HCN	0.3674E-02	0.5033E-02	0.6918E-02	0.8893E-02	0.1151E-01
11	H2O	0.4776E-05	0.3377E-05	0.2362E-05	0.1763E-05	0.1287E-05
12	OH	0.1048E-08	0.1567E-08	0.2371E-08	0.3315E-08	0.4720E-08
13	CO2	0.5516E-07	0.3656E-07	0.2401E-07	0.1709E-07	0.1191E-07
14	CO	0.4909E-01	0.4905E-01	0.4898E-01	0.4888E-01	0.4871E-01
15	CN	0.1288E-05	0.3571E-05	0.1013E-04	0.2345E-04	0.5659E-04
16	C2H	0.1635E-05	0.5675E-05	0.2030E-04	0.5684E-04	0.1681E-03
17	C3H	0.4827E-06	0.1860E-05	0.7403E-05	0.2259E-04	0.7315E-04
18	C4H	0.1909E-07	0.1005E-06	0.5484E-06	0.2162E-05	0.9161E-05
19	C3	0.4683E-10	0.3599E-09	0.2876E-08	0.1545E-07	0.9072E-07
20	C	0.1303E 01	0.1299E 01	0.1293E 01	0.1284E 01	0.1271E 01

# INDEPTH FLOW ANALYSIS(EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0061	0.0062	0.0062	0.0063	0.0063
TEMPERATURE (OF)	4104.5	4329.2	4595.6	4943.1	5505.7
PRESSURE (LB/FT2)	2162.9	2162.4	2161.8	2161.1	2160.0
MASS FLUX(LB/FT2-SEC)	0.0280	0.0296	0.0325	0.0399	0.0748

## GAS COMPONENT

## COMPOSITION (MOLE/MOLE GAS)

1	H	0.2724E-01	0.4460E-01	0.7484E-01	0.1323E 00	0.2530E 00
2	H2	0.8699E 00	0.8431E 00	0.7961E 00	0.7019E 00	0.4511E 00
3	CH3	0.9046E-04	0.1142E-03	0.1413E-03	0.1651E-03	0.1359E-03
4	CH4	0.9967E-04	0.7707E-04	0.5593E-04	0.3437E-04	0.1034E-04
5	C2H2	0.1217E-01	0.1916E-01	0.3043E-01	0.4885E-01	0.7125E-01
6	C2H4	0.6882E-05	0.7004E-05	0.6804E-05	0.5840E-05	0.2759E-05
7	C2H6	0.4155E-09	0.3010E-09	0.1991E-09	0.1037E-09	0.1901E-10
8	N2	0.2666E-01	0.2446E-01	0.2157E-01	0.1751E-01	0.1086E-01
9	NH3	0.1305E-05	0.1057E-05	0.8019E-06	0.5170E-06	0.1724E-06
10	HCN	0.1451E-01	0.1808E-01	0.2222E-01	0.2648E-01	0.2671E-01
11	H2O	0.9476E-06	0.6833E-06	0.4677E-06	0.2796E-06	0.9765E-07
12	OH	0.6569E-08	0.9137E-08	0.1278E-07	0.1800E-07	0.2325E-07
13	CO2	0.8452E-08	0.5926E-08	0.4007E-08	0.2464E-08	0.1081E-08
14	CO	0.4844E-01	0.4798E-01	0.4711E-01	0.4520E-01	0.3923E-01
15	CN	0.1295E-03	0.2981E-03	0.7154E-03	0.1902E-02	0.6594E-02
16	C2H	0.4686E-03	0.1323E-02	0.3964E-02	0.1361E-01	0.6391E-01
17	C3H	0.2222E-03	0.6844E-03	0.2253E-02	0.8608E-02	0.4680E-01
18	C4H	0.3598E-04	0.1439E-03	0.6270E-03	0.3308E-02	0.2795E-01
19	C3	0.4881E-06	0.2700E-05	0.1685E-04	0.1383E-03	0.2438E-02
20	C	0.1250E 01	0.1217E 01	0.1154E 01	0.1012E 01	0.4824E 00

TABLE B-4. Listing of ABLATIN2 Program

C		ABL2	1
C		ABL2	2
C		ABL2	3
C	-----INDEPTH RESPONSE OF AN ABLATIVE COMPOSITE	ABL2	4
C	NON-EQUILIBRIUM FLOW ANALYSIS	ABL2	5
C	ABLATIN2 SYSTEM	ABL2	6
C		ABL2	7
C		ABL2	8
	REAL*8 Z22	ABL2	9
	COMMON/KA/S1(6),S2(6),S3(6),S4(6),S5(6),A11(6),A22(6),	ABL2	10
1	A33(6),A44(6),A55(6),FI(30),FII(30),GI(30),	ABL2	11
2	GII(30),AA(30,6),S6(6),A66(6),JCODE(6),CPMX1	ABL2	12
	COMMON/KR/AT(30),BI(30),CI(30),DI(30),EI(30),AII(30),	ABL2	13
1	BII(30),CII(30),DII(30),EII(30),TLOW(30)	ABL2	14
	COMMON/KC/ICODE(30),Y(30),FW(30)	ABL2	15
	COMMON/KCC/SPCIE1(30),SPCIE2(30),TABLE(300,26),Z,INDPT	ABL2	16
	COMMON/KE/XTKF(100),ZOMGA(100),EK(100),SIG(100)	ABL2	17
	COMMON/KEE/PL,RR,TZERO,EPS,KEY,NC,NS,MM,NQ	ABL2	18
	COMMON/KF/CPS,CDO,DCDO,JCHAR,TC	ABL2	19
	COMMON/KI/KN,K7,DTCC,REAC2,W,KMAX,AVGFW,N,Z2,DELZ,H	ABL2	20
	COMMON/KJ/DELTK,TVAR	ABL2	21
	COMMON/KK/WTOTAL,RHOII	ABL2	22
	COMMON/KM/XMOL(30)	ABL2	23
	COMMON/KQ/Z22	ABL2	24
	DIMENSION TI(300),ZX(41),ZY(41),TP(41),P(41),WFLUX(41),	ABL2	25
1	TT(21),YCOMP(30,41),PROD(21),PRODCP(21),CP(30),	ABL2	26
2	PRODR(21),COND(30),CV(30),VIS(30),YI(30),Z1(300),	ABL2	27
3	TOK(300),CHARDN(300)	ABL2	28
	DOUBLE PRECISION ZZ,H11,ZLL,TTTT,DTCC,REAC1,CPB1,CPB2	ABL2	29
	F(A)=+GROUP*A	ABL2	30
	G(A)=A	ABL2	31
C		ABL2	32
C	DELTF=CHANGE IN DF FOR AN INCREMENT OF CHANGE IN H(FFET)	ABL2	33
	RHO=13.	ABL2	34

C	WI=0.01	ABL2	35
C		ABL2	36
C	RR=GAS CONSTANT(1.98726BTU/(LB-MOLE OR)	ABL2	37
C	TZFRO=REFERENCE TEMPERATURE	ABL2	38
C	TFMAX=MAXIMUM ALLOWABLE TEMPERATURE FOR THIS MODEL (OF)	ABL2	39
C		ABL2	40
	RR=1.98726	ABL2	41
	TZERO=298.159	ABL2	42
C		ABL2	43
C	HSIMPI=SIMPSON'S RULE INCREMENT SIZE(FT) USED	ABL2	44
C	IN THE SOLUTION OF THE MOMENTUM EQUATION	ABL2	45
	FR2=778.16/32.2	ABL2	46
C		ABL2	47
C		ABL2	48
C	NC=NO. OF GAS SPECIES	ABL2	49
C	NNS=NO. OF LIQUID OR SOLID SPECIES	ABL2	50
C	NS=NC+NNS(TOTAL NUMBER OF SPECIES)	ABL2	51
C	MM=NO. OF ELEMENTS	ABL2	52
C	KODE=1 CONDUCTIVITY OF CHAR WITH GAS IN PORES	ABL2	53
C	INDPT=0 COMPUTATIONS START AT THE BACK SURFACE OF THE CHAR	ABL2	54
C	INDPT=1 COMPUTATIONS START AT THE VIRGIN MATERIAL	ABL2	55
C	PL=PRESSURE AT Z=L(LB/FT <sup>2</sup> )	ABL2	56
C	DELTK=TEMPERATURE INCREMENT	ABL2	57
C	TD=TEMPERATURE AT Z=0	ABL2	58
C	EPS=POROSITY	ABL2	59
C	ZL=ABLATOR THICKNESS(IN FEET)	ABL2	60
C	HI=INITIAL RUNGE-KUTTA INCREMENT SIZE(FT) USED	ABL2	61
C	IN THE SOLUTION OF THE ENERGY EQUATION.	ABL2	62
C	ALPHA=VISCOUS COEFFICIENT IN DARCY'S EQUATION(1/FT)	ABL2	63
C	BETA=INERTIAL COEFFICIENT IN DARCY'S EQUATION(1/FT <sup>2</sup> )	ABL2	64
C	SIGMA=STEPHAN-BOLTZMAN CONSTANT(0.481X10 <sup>-12</sup> BTU/FT <sup>2</sup> -SEC-OF4)	ABL2	65
C	EMIS=CHAR EMISIVITY.	ABL2	66
C	QFLUXI=INITIAL BACK SURFACE HEAT FLUX.	ABL2	67
C	QINC=INCREMENT IN THE HEAT FLUX(FOR PARAMETER STUDIES)	ABL2	68

C	QMAX=MAXIMUM BACK SURFACE HEAT FLUX.	ABL2	69
C	TCHAR=BACK SURFACE TEMPERATURE OF CHAR	ABL2	70
C		ABL2	71
C		ABL2	72
	FR=0.1666667	ABL2	73
C		ABL2	74
C		ABL2	75
C	-----READ INPUT PARAMETERS	ABL2	76
C		ABL2	77
C		ABL2	78
C		ABL2	79
10	READ11,NC,NNS,MM,KODE,KEY,INDPT,TMAX	ABL2	80
11	FORMAT(6I6,F10.1)	ABL2	81
	READ 12,PL,TO,FPS,ZL,HI	ABL2	82
12	FORMAT(F10.3,10X,4F10.3)	ABL2	83
	READ21,ALPHA,BETA,SIGMA,EMIS	ABL2	84
	READ13,DTC,TCHAR,VR	ABL2	85
13	FORMAT(7E10.3)	ABL2	86
	NN=NC	ABL2	87
	NS=NC+NNS	ABL2	88
	NQ=NS	ABL2	89
C		ABL2	90
C		ABL2	91
C		ABL2	92
C	S1...S6(APPLY BETWEEN 1000-6000 OK)	ABL2	93
C	A11...A66(APPLY BETWEEN 300-1000 OK)	ABL2	94
C	JCODE(J)=0 THE REFERENCE ELEMENT IS IN THE GAS STATE.	ABL2	95
C	JCODE(J)=1 THE REFERENCE ELEMENT IS IN THE SOLID STATE.	ABL2	96
C	AI...EI(HEAT CAPACITY CONSTANTS...1000-6000 OK)	ABL2	97
C	FI,GI(NEEDED TO CALCULATE THE ENTHALPY,ENTROPY	ABL2	98
C	AND FREE ENERGY....1000-6000 OK)	ABL2	99
C	AII...GII(300-1000 OK)	ABL2	100
C	AA=FORMULA NUMBER. GIVES THE ATOMS OF ELEMENT J	ABL2	101
C	IN SPECIE I.	ABL2	102



C	TLOW(I)=MINIMUM TEMPERATURE AT WHICH THE HIGH TEMPERATURE	ABL2 103
C	FIT IS APPLICABLE.	ABL2 104
C	FW(I)=MOLECULAR WEIGHT OF SPECIE I.	ABL2 105
C	YI(I)=INITIAL MOLE FRACTION OF SPECIE I.	ABL2 106
C	YI(I)=MOLE FRACTION OF SPECIF I.	ABL2 107
C	SPCIF1 AND SPCIE2 ARE THE SPECIES IDENTIFICATION	ABL2 108
C	ICODE(I)=0 SPECIE IS A GAS	ABL2 109
C	ICODE(I)=1 SPECIE IS A SOLID	ABL2 110
C		ABL2 111
C		ABL2 112
C		ABL2 113
C		ABL2 114
C	-----READ EMPIRICAL CONSTANTS TO CALCULATE THE SENSIBLE	ABL2 115
C	ENTHALPY CHANGE OF THE CONSTITUENT ELEMENTS.	ABL2 116
C		ABL2 117
C		ABL2 118
	DO 9 J=1,MM	ABL2 119
	READ 18,S1(J),S2(J),S3(J),S4(J),S5(J),S6(J),JCODE(J)	ABL2 120
	READ 18,A11(J),A22(J),A33(J),A44(J),A55(J),A66(J)	ABL2 121
9	CONTINUE	ABL2 122
	DO15I=1,NS	ABL2 123
	READ 14,TLOW(I),FW(I),YI(I),SPCIF1(I),SPCIE2(I),ICODE(I)	ABL2 124
14	FORMAT(10X,3E10.3,2X,2A3,I4)	ABL2 125
C		ABL2 126
C		ABL2 127
C	-----READ EMPIRICAL CONSTANTS TO CALCULATE THE HEAT	ABL2 128
C	CAPACITY OF THE SOLID PLUS TWO ADDITIONAL CONSTANTS	ABL2 129
C	TO CALCULATE THE ENTHALPY,THE ENTROPY AND THE FREE	ABL2 130
C	ENERGY OF THE SYSTEM	ABL2 131
C		ABL2 132
C		ABL2 133
	READ13,AI(I),BI(I),CI(I),DI(I),EI(I),FI(I),GI(I)	ABL2 134
	READ13,AII(I),BII(I),CII(I),DII(I),FII(I),FIII(I),GII(I)	ABL2 135
C		ABL2 136

C		ABL2 137
15	READ13,(AA(I,J),J=1,MM)	ABL2 138
C		ABL2 139
C		ABL2 140
C		ABL2 141
C	EK=POTENTIAL PARAMETER/BOLTZMAN CONSTANT.	ABL2 142
C	SIG=COLLISION DIAMETER(ANGSTRONG UNITS).	ABL2 143
C	THESE CONSTANTS ARE USED TO DETERMINE THE	ABL2 144
C	VISCOCITY AND THERMAL CONDUCTIVITY OF THE	ABL2 145
C	REACTING GAS MIXTURE.	ABL2 146
C	NDATA=NO. OF XTKE VS. ZOMGA DATA POINTS	ABL2 147
C	XTKE=PRODUCT OF TEMPERATURE AND 1/EK VALUE	ABL2 148
C	ZOMGA=COLLISION INTEGRAL TABULATED VS XTKE	ABL2 149
C		ABL2 150
C		ABL2 151
C		ABL2 152
	READ16,(FK(I),SIG(I),I=1,NC)	ABL2 153
16	FORMAT(2F15.5)	ABL2 154
	READ11,NDATA	ABL2 155
	READ17,(XTKE(I),ZOMGA(I),I=1,NDATA)	ABL2 156
17	FORMAT(2F15.5)	ABL2 157
18	FORMAT(6E10.4,I3)	ABL2 158
21	FORMAT(3E15.5,F15.5)	ABL2 159
C		ABL2 160
C		ABL2 161
C	-----INITIALIZATION OF PARAMETERS	ABL2 162
C		ABL2 163
C		ABL2 164
C	N=COUNTER OF RUNGE KUTTA STEPS	ABL2 165
	N=1	ABL2 166
	K7=1	ABL2 167
C	K7=1(CALL SUBPROGRAM INPUT)K7=2(RYPASS SUBPROGRAM	ABL2 168
C	INPUT)	ABL2 169
C		ABL2 170

C	TO=INITIAL TEMPERATURE OF BACK SURFACE(OF)	ABL2	171
C	IT IS A SPECIFIED BOUNDARY CONDITION.	ABL2	172
C	TC=INSTANTANEOUS TEMPERATURE OF THE SYSTEM(OF)	ABL2	173
C	K1=1	ABL2	174
C	K1=GIVES THE TOTAL NUMBER OF DATA POINTS STORED.	ABL2	175
C	SHOULD NOT EXCEED THE DIMENSION OF VARIABLES.	ABL2	176
C		ABL2	177
	NN4=NC+4	ABL2	178
	NN5=NN4+NNS	ABL2	179
C		ABL2	180
C		ABL2	181
C	NN5 GIVES THE NUMBER OF VARIABLES STORED IN TABLE(I,J).	ABL2	182
C	THE FIRST FOUR VARIABLES ARE...	ABL2	183
C	1) THE TEMPERATURE(IN OK)	ABL2	184
C	2) THE HEAT ABSORBED BY REACTIONS(BTU/FT2-SEC)	ABL2	185
C	3) THE AVERAGE MOLECULAR WEIGHT	ABL2	186
C	4) THE MASS FLUX(LBS/FT2-SEC)	ABL2	187
C	5) THE REST OF THE VARIABLES ARE THE MOLE	ABL2	188
C	FRACTIONS. FOR THE SOLIDS, THE TERM STORED	ABL2	189
C	IS THE RATIO OF MOLES OF SOLID TO MOLE OF	ABL2	190
C	GASES.	ABL2	191
C		ABL2	192
C		ABL2	193
C		ABL2	194
C	-----CONVERT INITIAL COMPOSITION OF THE GASES TO MOLE	ABL2	195
C	FRACTION AND CALCULATE THE RATIO OF THE MOLES OF	ABL2	196
C	EACH SOLID SPECIE PER MOLE OF THE GAS MIXTURE. THIS	ABL2	197
C	IS DONE IN CASE THE YI(I) IS READ IN AS MOLES.	ABL2	198
C		ABL2	199
C	ZL=THICKNESS OF CHAR IN INCHES	ABL2	200
	ZL=ZL/12.	ABL2	201
	ZINC=ZL/98.	ABL2	202
	ZINC=ZINC/5.	ABL2	203
	IF(VR.GE.1.F-2)ZINC=ZINC/2.	ABL2	204

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      IF(VR.GE.2.F-2)ZINC=ZINC/2.
22  IND=0
      KMAX=0
      KID=0
      DELTFF=0.
      REAC1=0.
      CPB1=0.
      CPB2=0.
      Q1=0.
      DCDO=0.
      DCDOV=0.
      DELTK=0.
      K1=1
      TC=T0
      SUM=0.
      DO23I=1,NC
23  SUM=SUM+YI(I)
      DO24I=1,NS
24  YI(I)=YI(I)/SUM
C
C
C      HI=INITIAL RUNGE-KUTTA STEP SIZE
C
C      H=HI
C
C
C-----CALCULATE THE INITIAL AVERAGE MOLECULAR WEIGHT OF THE GAS
C
C
      AVGEFW=0.
      DO31I=1,NS
      XMOL(I)=YI(I)
      Y(I)=YI(I)
      IF(ICODE(I).EQ.1)GOTO31

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31	AVGFW=AVGFW+Y(I)*FW(I)	ABL2	239
	CONTINUE	ABL2	240
C	W=MASS FLUX(LBS-FT2/SEC)	ABL2	241
	W=WI	ABL2	242
	Z=0.	ABL2	243
C	Z=DISTANCE IN FEET	ABL2	244
	Z2=0.	ABL2	245
	Z22=Z2	ABL2	246
	TVAR=(TC+459.69)/1.8	ABL2	247
C	TVAR=TEMPERATURE IN OK.	ABL2	248
	ZZ=0.	ABL2	249
	ZLL=ZL	ABL2	250
	PRINT 51,ZLL	ABL2	251
	51 FORMAT(1X,'ZLL='D20.9)	ABL2	252
C		ABL2	253
C		ABL2	254
C		ABL2	255
C		ABL2	256
C	-----INDEPTH RESPONSE OF ABLATIVE COMPOSITES.	ABL2	257
C	FOR BACK SURFACE TEMPERATURE AND HEAT	ABL2	258
C	FLUX SPECIFIED. THE EQUATION OF ENERGY	ABL2	259
C	IS A SECOND ORDER, NON-LINEAR, ORDINARY DIFFERENTIAL	ABL2	260
C	EQUATION WITH VARIABLE COEFFICIENTS.	ABL2	261
C		ABL2	262
C	THE NUMERICAL TECHNIQUE USED IS A 4TH ORDER	ABL2	263
C	VARIABLE STEP RUNGE-KUTTA ANALYSIS.	ABL2	264
C		ABL2	265
C		ABL2	266
C	TCHAR=TEMPERATURE AT WHICH ALL OF THE VIRGIN	ABL2	267
C	MATERIAL HAS DECOMPOSED.	ABL2	268
C		ABL2	269
	DEL7=H	ABL2	270
	H11=H	ABL2	271
	IF(TVAR.GT.TCHAR)GOTO32	ABL2	272

C	CALL INDPHT(TC,CDOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,DELTK,	ABL2 273
	IN,DELZ,VR,W,H)	ABL2 274
	H11=H	ABL2 275
	DELZ=H	ABL2 276
C		ABL2 277
C	CDOV=THERMAL CONDUCTIVITY OF VIRGIN MATERIAL (	ABL2 278
C	BTU/(FT-SEC-OF)	ABL2 279
C	DCDOV=THE DERIVATIVE OF CDOV WITH TEMPERATURE(BTU/(FT-2EC))	ABL2 280
C	GASCP=HEAT CAPACITY OF MIXTURE(BTU/LB-OF)	ABL2 281
C	Q=HEAT ABSORBED BY DEPOLYMERIZATION OF THE	ABL2 282
C	VIRGIN PLASTIC COMPOSITE(BTU/FT3-SEC)	ABL2 283
C	CPV=HEAT CAPACITY OF VIRGIN COMPOSITE(BTU/LB-OF)	ABL2 284
C	RHO=DENSITY OF VIRGIN COMPOSITE	ABL2 285
C	DELTK=TEMPERATURE DIFFERENCE IN OK FOR A DISTANCE H.	ABL2 286
C	N=NUMBER OF INTEGRATION STEPS	ABL2 287
C	DELZ=INCREMENT OF DISTANCE(FT)	ABL2 288
C	VR=SURFACE RECESSION VELOCITY(FT/SEC)	ABL2 289
C	W=MASS FLUX(LBS/FT2-SEC)	ABL2 290
C	H=RUNGE-KUTTA INTEGRATION STEP SIZE(FT)	ABL2 291
C	DTC=QFLUX/CDOV	ABL2 292
C		ABL2 293
	WI=W	ABL2 294
	DTCI=DTC	ABL2 295
	QCZI=CDOV*DTC	ABL2 296
	PRINT 1390,QCZI	ABL2 297
	1390 FORMAT(1X,'QCZ='F15.5)	ABL2 298
C		ABL2 299
C		ABL2 300
C	-----CALCULATE THE HEAT CAPACITY OF THE PYROLYSIS GASFS	ABL2 301
C		ABL2 302
C		ABL2 303
	CALL CPMIX(TVAR,NN,CPMX)	ABL2 304
	GASCP=CPMX/AVGEW	ABL2 305
		ABL2 306

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      GOTO113
C
  32  CALL CHARPR
C
C-----THIS SUBROUTINE CALCULATES THE THERMO-PHYSICAL
C      PROPERTIES IN THE CHAR
C
      DELZ=H
      Z1(1)=0.
      T1(1)=T0
      DTC=QFLUX1/COO
      PRINT 36,COO
  36  FORMAT(1X,'COO='E15.6)
      DTCI=DTC
      GOTO103
  101  TVAR=(TC+459.69)/1.8
C
C
      IF(TVAR.GT.TCHAR)GOTO102
C
C
C-----CALCULATE THE PHYSICO-CHEMICAL PROPERTIES AND DESCRIBE
C      THE DECOMPOSITION OF THE VIRGIN MATERIAL USING INDPH.
C
C
      CALL INDPH(TC,COOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,DELTK,
      IN,DELZ,VR,W,H)
C
C      FOR EXPLANATION OF THE VARIABLES IN THE ARGUMENT SEE
C      PREVIOUS CALL INDPH STATEMENT.
C
      H11=H
      W1=W
      ZLL=ZZ+.0208333

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ABL2 340

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PRINT 139,TC,TVAR,DTC,GASCP,DCDOV,CPV,Q,CDOV,Z7	ABL2 341
139 FORMAT(1X,'T='F9.4,' TK='F9.4,' DT='E11.4,' CP='F6.3,' DKE='E11.4,	ABL2 342
1' CPP='E11.4,' Q='E11.4,' KE='E11.4,D15.7)	ABL2 343
QCZI=CDOV*DTC	ABL2 344
PRINT 1390,QCZI	ABL2 345
C	ABL2 346
C	ABL2 347
C-----CALCULATE THE HEAT CAPACITY OF THE PYROLYSIS GASES	ABL2 348
C	ABL2 349
C	ABL2 350
CALL CPMIX(TVAR,NN,CPMX)	ABL2 351
GASCP=CPMX/AVGEW	ABL2 352
GOTO113	ABL2 353
C	ABL2 354
C	ABL2 355
C-----USE SUBROUTINE CHARPR TO GENERATE NEEDED PHYSICAL PROPERTY	ABL2 356
C DATA FOR THE CHAR ZONE(HEAT CAPACITY OF THE CHAR AND THE	ABL2 357
C OVER ALL EFFECTIVE THERMAL CONDUCTIVITY OF THE GAS AND CHAR).	ABL2 358
C	ABL2 359
C	ABL2 360
102 CALL CHARPR	ABL2 361
IF(IND.EQ.0)DTC=QCZI/CDO	ABL2 362
IND=1	ABL2 363
C	ABL2 364
C	ABL2 365
C-----CALCULATE THE BULK DENSITY OF THE CHAR	ABL2 366
C	ABL2 367
C	ABL2 368
C	ABL2 369
C ROCHAR=BULK DENSITY OF THE CHAR(LBS/FT**3)	ABL2 370
ROCHAR=(WTOTAL-W)/VR	ABL2 371
C	ABL2 372
DELZ=H	ABL2 373
C	ABL2 374



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C
C-----CALCULATE THE CHEMICAL KINETICS OF THE PYROLYSIS GASES
C      AND CHAR ALONG WITH THE HEAT ABSORB BY THESE REACTING
C      GASES USING KINET.
C
C
103  CALL KINET
      H11=H
      GASCP=CPMX1/AVGFW
C
C
C-----CALCULATE THE GROUP TERM
C
C
112  REACT=REAC2/DTC
      CONVEG=W*GASCP
      CPB1=CPB1+CONVEG*DELTF
      CONVES=CPS*RHOCHAR*VR
      CPB2=CPB2+CONVES*DELTF
      REAC1=REAC1+REACT*DELTF
      GROUP=(CONVEG+CONVES-DCDO*DTC+REACT)/CDO
C
C
C      DCDO=DERIVATIVE OF CDO WITH TEMPERATURE(BTU/FT-SEC-OF2)
C      CDO=EFFECTIVE THERMAL CONDUCTIVITY(BTU/FT-SEC-OF)
C      DTC=GRADIENT OF TEMPERATURE WITH DISTANCE(OF/FT)
C      VR=SURFACE RECESSION VELOCITY(FT/SEC)
C
C
      GOTO114
113  Q2=Q/DTC
      IF(Q2.LT.0.)Q2=0.
      CONVEG=W*GASCP
      CONVEV=CPV*RHO*VR

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ABL2 408

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      Q1=Q1+Q2*DELTF
      GROUP=(CONVEG+CONVEV-DCDOV*DTC+Q2)/CDOV
C
C
C-----THE ABOVE GROUP TERM IS USED DURING THE DEPOLYMERIZATION OF
C      THE VIRGIN PLASTIC COMPOSITE.
C
C
114  A=DTC
      DT=A
      ARK=H*DT
      A1=ARK
      DA1=ARK*GROUP
      DT=A+0.5*DA1
      ARK=H*DT
      A2=ARK
      DA2=ARK*GROUP
      DT=A+0.5*DA2
      ARK=H*DT
      A3=ARK
      DA3=ARK*GROUP
      DT=A+DA3
      ARK=H*DT
      A4=ARK
      DA4=ARK*GROUP
      DTC=DTC+(DA1+2.*(DA2+DA3)+DA4)/6.
      IF(IND.EQ.0)GOTO115
      QCZ=CDO*DTC
115  TPREV=TC
      IF(H.LT.0.8E-8)GOTO117
      TC=TC+(A1+2.*(A2+A3)+A4)/6.
      GOTO118
117  IF(K10.EQ.0)TTTT=TC
      K10=1

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ABL2 409
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DTCC=DTC	ABL2 443
TITT=TITT+H11*DTCC	ABL2 444
TC=TITT	ABL2 445
118 DELTFF=TC-TPREV	ABL2 446
DELTK=DELTFF/1.8	ABL2 447
C	ABL2 448
C	ABL2 449
C-----COMPARE THE TEMPERATURE CALCULATED WITH THE MAXIMUM VALUE.	ABL2 450
C	ABL2 451
C	ABL2 452
138 ZPREV=ZZ	ABL2 453
ZZ=Z7+H11	ABL2 454
H11=H	ABL2 455
Z=ZZ	ABL2 456
IF(TC.GT.TFMAX)GOTO150	ABL2 457
N=N+1	ABL2 458
IF(TVAR.LE.TCHAR)Z2=ZZ	ABL2 459
IF(TVAR.LE.TCHAR)GOTO101	ABL2 460
IF(Z2.GT.ZZ)GOTO101	ABL2 461
140 PRINT 142,TC,H,DTC,GASCP,DCDD,GROUP,REACT,CDD	ABL2 462
142 FORMAT(1X,'TF='F9.4,' H='E14.6,' DT='E11.5,' CP='F6.4,' DKE='F11	ABL2 463
1.5,' GRP='E12.5,' Q='E11.4,' KE='E11.5)	ABL2 464
PRINT 1140,AVGEW,W, TVAR,KMAX,CPS,GASCP,RHO,QCZ	ABL2 465
1140 FORMAT(1X,'AVGEW='F 7.3,' W='F 7.5,' TVAR='F7.2,	ABL2 466
1' KMAX='F5,' CPS='F 6.3,' GASCP='F 6.4,' RHO='F8.4,' QC7='F7.2 )	ABL2 467
Z2=Z2+ZINC	ABL2 468
Z1(K1)=ZPREV	ABL2 469
TOK(K1)=TVAR	ABL2 470
T1(K1)=TPREV	ABL2 471
CHARDN(K1)=ROCHAR	ABL2 472
C	ABL2 473
C	ABL2 474
C-----STORE THE TEMPERATURE PROFILE FOR LATER USE IN THE SOLUTION	ABL2 475
C OF THE MOMENTUM EQUATION.	ABL2 476

C		ABL 2 477
C		ABL 2 478
	PRINT 153,REAC1,CPB1,CPB2,ZPREV	ABL 2 479
153	FORMAT(1X,'REAC1='D15.7,' CPB1='D15.7,' CPB2='D15.7,	ABL 2 480
	1' ZPREV='E15.7/)	ABL 2 481
	K1=K1+1	ABL 2 482
	IF(K1.GE.299)K1=299	ABL 2 483
C		ABL 2 484
C	THE NUMBER OF DIMENSIONES OF TABLE,T1 AND Z1.	ABL 2 485
C		ABL 2 486
C	-----K1 SHOULD NEVER BE GREATER THAN 299 TO AVOID VIOLANTING THE	ABL 2 487
	GOTO101	ABL 2 488
C		ABL 2 489
150	TL=TC	ABL 2 490
	WFINAL=W	ABL 2 491
C	TL=FINAL TEMPERATURE	ABL 2 492
	PRINT 1140,AVGEW,W, TVAR,KMAX,CPS,GASCP,RHO,QCZ	ABL 2 493
	PRINT 142,TC,H,DTC,GASCP,DCDD,GROUP,REACT,CDD	ABL 2 494
	PRINT 153,REAC1,CPB1,CPB2,ZPREV	ABL 2 495
	TOK(K1)=(TC+459.69)/1.8	ABL 2 496
	T1(K1)=TL	ABL 2 497
	CHARDN(K1)=ROCHAR	ABL 2 498
C		ABL 2 499
C	*****	ABL 2 500
C	*****	ABL 2 501
C		* ABL 2 502
C	-----THE TEMPERATURE PROFILE HAS BEEN DEFINED	* ABL 2 503
C		* ABL 2 504
C	*****	ABL 2 505
C	*****	ABL 2 506
C		ABL 2 507
	DELTT=TL-T1(1)	ABL 2 508
C	DELTT=TEMPERATURE DROP ACROSS THE CHAR(OF)	ABL 2 509
	Z1(K1)=ZZ	ABL 2 510

```

C
C
C-----PRINT THE TEMPERATURE AND THE DENSITY PROFILE
C
C
      PRINT 154
154  FORMAT(1H1, 7X,'T(OF)', 9X,'T(OK)', 11X,'Z')
      DO 156 I=1,K1
      PRINT 155,T1(I),TOK(I),Z1(I)
155  FORMAT(1X,4E15.7)
156  CONTINUE
      DISTAN=Z1(K1)-Z1(1)
C
C      DISTAN IS THE THICKNESS OF THE CHAR.
C      CALCULATION OF THE PRESSURE PROFILE IN THE
C      CHAR USING STIMPSON'S RULE FOR THE INTEGRATION
C      OF THE MOMENTUM EQUATION FOLLOWS.
C
      JS=39
C
C      JS=NUMBER OF SLICES IN THE CHAR
C
      HS=DISTAN/FLOAT(JS)
C
C      HS=INCREMENT OF GRID(IN FEET)
C
C
C-----INITIALIZE
C
C
      SIMP1=0.
      SIMP2=0.
      ITEMP=K1
C

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ABL2 511
ABL2 512
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ABL2 544

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C	ITEMP=TOTAL NUMBER OF TEMPERATURE POINTS STORED	ABL2 545
C		ABL2 546
	LS=JS+1	ABL2 547
	WFLUX(1)=WT	ABL2 548
	ZX(LS)=Z1(K1)	ABL2 549
	TP(LS)=TL	ABL2 550
	P(LS)=PL	ABL2 551
C		ABL2 552
C		ABL2 553
C	-----THE INTEGRATION OF THE MOMENTUM EQUATION IS PERFORMED	ABL2 554
C		ABL2 555
C		ABL2 556
C		ABL2 557
C	-----FROM THE FRONT SURFACE OF THE CHAR TO THE BACK SURFACE.	ABL2 558
C	THE INTEGRATION OF THE ENERGY EQUATION, ON THE OTHER	ABL2 559
C	HAND, WAS PERFORMED FROM THE VIRGIN MATERIAL TO THE FRONT	ABL2 560
C	SURFACE OF THE CHAR. BECAUSE THE DIRECTION OF INTEGRATION	ABL2 561
C	OF BOTH EQUATIONS ARE DIFFERENT IT IS NECESSARY TO RE-	ABL2 562
C	DEFINE Z=0. AT THE FRONT SURFACE OF THE CHAR.	ABL2 563
C		ABL2 564
C		ABL2 565
	ACON1=2.6693E-3	ABL2 566
	ACON5=2.42/3600.	ABL2 567
	ACON7=778.16/32.2	ABL2 568
	MS=20	ABL2 569
	HSMPI=HS/FLOAT(MS)	ABL2 570
	MP=MS+1	ABL2 571
	DO260N=1,JS	ABL2 572
	NBAR=N-1	ABL2 573
	HN=NBAR	ABL2 574
	LO=LS-NBAR	ABL2 575
	ZX(LO)=ZX(LS)-HN*HS	ABL2 576
	ZY(MP)=ZX(LO)	ABL2 577
C		ABL2 578

C-----DEFINE MP AS THE TOTAL NO. OF POINT OVER WHICH SIMPSON'S  
C RULE IS TO BE APPLIED  
C

DO241M=1,MP  
MBAR=M-1  
HM=MBAR  
MD=MP-MBAR  
ZY(MD)=ZY(MP)-HM\*HSIMP1  
ZVAR=ZY(MD)  
IF(ZVAR.LE.Z1(1))ZVAR=Z1(1)

C  
C

C-----FOR A SPECIFIED CHAR DISTANCE OBTAIN THE  
C CORRESPONDING TEMPERATURE FROM THE TEMPE-  
C RATURE PROFILE  
C

CALL INTRPL(ZVAR,Z1,T1,ITEMP,TVIS)

C

C TVIS IS THE INTERPOLATED TEMPERATURE IN OF  
C WHICH CORRESPONDS TO THE VALUE OF ZVAR  
C

TK=(459.69+TVIS)/1.8

C

C TK=TEMPERATURE IN KELVIN  
C

DO205I=1,NC  
TKE=TK/EK(I)

C

C

C-----FOR THE VALUE OF INTERPOLATED TEMPERATURE FIND  
C THE CORRESPONDING COLLISION INTEGRAL TO CALCULATE  
C THE PURE GAS VISCOSITY USING THE METHOD OF WILKE-JOHNSON  
C

C

C

ABL2 579  
ABL2 580  
ABL2 581  
ABL2 582  
ABL2 583  
ABL2 584  
ABL2 585  
ABL2 586  
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ABL2 608  
ABL2 609  
ABL2 610  
ABL2 611  
ABL2 612

CALL INTRPL(TKE,XTKE,ZOMGA,NDATA,OMGA)	ABL2 613
C	ABL2 614
C OMGA=COLLISION INTEGRAL	ABL2 615
C	ABL2 616
205 VIS(I)=2.6693E-3*SQRT(FW(I)*TK)/(SIG(I)**2*OMGA)	ABL2 617
206 TVAR=TK	ABL2 618
DD218KL=3,NN5	ABL2 619
C	ABL2 620
C	ABL2 621
C-----INTERPOLATE FOR THE DATA GENERATED IN KINET	ABL2 622
C	ABL2 623
C	ABL2 624
CALL INTRPL(TVAR,TABLE(1,1),TABLE(1,KL),KMAX,VARY)	ABL2 625
IF(KL.GT.4)GOTO216	ABL2 626
C	ABL2 627
C KMAX=NUMBER OF DATA POINTS STORED	ABL2 628
C	ABL2 629
IF(KL.EQ.4)GOTO215	ABL2 630
AVGFW=VARY	ABL2 631
GOTO218	ABL2 632
215 W=VARY	ABL2 633
GOTO218	ABL2 634
216 Y(KL-4)=VARY	ABL2 635
IF(VARY.GT.0.)GOTO217	ABL2 636
Y(KL-4)=1.E-70	ABL2 637
217 IF(M.GT.1)GOTO218	ABL2 638
TP(LO)=TVIS	ABL2 639
WFLUX(LO)=W	ABL2 640
KYCOMP=KL-4	ABL2 641
YCOMP(KYCOMP,LO)=Y(KYCOMP)	ABL2 642
218 CONTINUE	ABL2 643
VMIX=0.	ABL2 644
DD236J=1,NC	ABL2 645
TERM=1.	ABL2 646



DO230L=1,NC	ABL2 647
IF(L.EQ.J)GOTO230	ABL2 648
TOPV=(1.+SQRT(VIS(J)/VIS(L))*SQRT(SQRT(FW(L)/FW(J))))**2	ABL2 649
BOTV= SQRT(2.)*SQRT(1.+FW(J)/FW(L))*2.	ABL2 650
PHIV=TOPV/BOTV	ABL2 651
TERM=TERM+PHIV*(Y(L)/Y(J))	ABL2 652
230 CONTINUE	ABL2 653
VMIX=VMIX+VIS(J)/TERM	ABL2 654
236 CONTINUE	ABL2 655
C ACON5=2.42/3600.	ABL2 656
238 VISCONS=VMIX*ACON5	ABL2 657
239 PRD(MD)=TVIS*VISCONS*W/AVGEW	ABL2 658
TT(MD)=TVIS/AVGEW*(W**2)	ABL2 659
241 CONTINUE	ABL2 660
ZX(LD-1)=ZX(LD)-HS	ABL2 661
C	ABL2 662
C-----COMMENCE SIMPSON'S RULE INTEGRATION	ABL2 663
C	ABL2 664
SUM1=0.	ABL2 665
SUM2=0.	ABL2 666
SUM3=0.	ABL2 667
SUM4=0.	ABL2 668
MODD=MP-2	ABL2 669
DO255KP=3,MODD,2	ABL2 670
SUM1=SUM1+2.*PRD(KP)	ABL2 671
255 SUM3=SUM3+2.*TT(KP)	ABL2 672
MEVEN=MP-1	ABL2 673
DO256KP=2,MEVEN,2	ABL2 674
SUM2=SUM2+4.*PRD(KP)	ABL2 675
256 SUM4=SUM4+4.*TT(KP)	ABL2 676
SIMP1=(HSIMP1/3.0)*(PRD(1)+SUM1+SUM2+PRD(MP))+SIMP1	ABL2 677
SIMP2=(HSIMP1/3.0)*(TT(1)+SUM3+SUM4+TT(MP))+SIMP2	ABL2 678
C FR2=778.16/32.2	ABL2 679
P(LD-1)=SQRT(PL**2+(2.*RR)*FR2*(ALPHA*SIMP1+BETA*SIMP2))	ABL2 680

260	CONTINUE	ABL2	681
C		ABL2	682
C		ABL2	683
C	-----CALCULATE THE SURFACE HEAT FLUX,QL,THE RERADIATION,QR,	ABL2	684
C	AND THE TOTAL AERODYNAMIC HEATING,QA.	ABL2	685
C		ABL2	686
C		ABL2	687
261	QL=QCZ	ABL2	688
262	QR=EMIS*SIGMA*(TL+459.69)**4	ABL2	689
	QA=QL+QR	ABL2	690
C		ABL2	691
	TP(1)=T1(1)	ABL2	692
C		ABL2	693
C	-----PRINT OUTPUT	ABL2	694
C		ABL2	695
2603	PRINT 597	ABL2	696
597	FORMAT(1H1/////////)	ABL2	697
5982	PRINT 5984	ABL2	698
5984	FORMAT(35X,'INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)')//)	ABL2	699
5986	PRINT 5990	ABL2	700
5990	FORMAT(12X,51H	THEORETICAL/ABL2	701
	1/)	ABL2	702
	PRINT600,T1(1),NC	ABL2	703
600	FORMAT(18X,'CHAR BACK TEMPERATURE (OF)='F7.1,13X,'NUMBER OF GAS COABL2	704	
	1MPONENTS='I3/)	ABL2	705
	THICK=DISTAN*12.	ABL2	706
	THICK1=Z1(1)*12.	ABL2	707
	PRINT 602,THICK,THICK1	ABL2	708
602	FORMAT(18X,'THICKNESS OF CHAR(INCHES)='F8.6,6X,'THICKNESS OF DECOMABL2	709	
	1POSITION ZONE='F8.6/)	ABL2	710
	QC7Z=QCZ-QC7I	ABL2	711
	PRINT 604,WTOTAL,WFLUX(LS)	ABL2	712
604	FORMAT(18X,'TOTAL MASS FLUX(LBS/FT2-SEC)='F7.6,6X,29HGAS MASS FLUXABL2	713	
	1 AT THE SURFACE=,1X,F7.6/)	ABL2	714

PRINT 611,TFMAX,VR	ABL2 715
611 FORMAT(18X,'FRONT SURFACE TEMPERATURE(OF)='F6.1,5X,'SURFACE RECESSABL2 716	
ION VELOCITY(FT/SEC)='F7.5/)	ABL2 717
PRINT 603,QCZZ,QCZI	ABL2 718
603 FORMAT(25X,'RATE OF HEAT ABSORBED IN THE CHAR ZONE(BTU/FT2-SFC)=' ABL2 719	
1F9.4, //25X,'RATE OF HEAT ABSORBED IN THE DECOMPOSITION ZONE(BTU/FTABL2 720	
22-SFC)='F9.4/)	ABL2 721
HCHAR=QCZZ/QCZ*100.	ABL2 722
HDECOM=QCZI/QCZ*100.	ABL2 723
SUM=REAC1+CPB1+CPB2	ABL2 724
HGAS=CPB1/SUM*100.	ABL2 725
HSOLID=CPB2/SUM*100.	ABL2 726
HREACT=REAC1/SUM*100.	ABL2 727
PRINT 605,HCHAR	ABL2 728
605 FORMAT(25X,'PERCENT OF TOTAL HEAT ABSORBED IN THE CHAR ZONE='E15.7ABL2 729	
1/)	ABL2 730
PRINT 606,HDECOM	ABL2 731
606 FORMAT(25X,'PERCENT OF TOTAL HEAT ABSORBED IN DECOMP-ZONE='E15.7/)	ABL2 732
PRINT 607,HGAS	ABL2 733
607 FORMAT(25X,'PERCENT OF HEAT ABSORBED BY THE GAS IN THE CHAR ZONE='ABL2 734	
1E15.7/)	ABL2 735
PRINT 608,HSOLID	ABL2 736
608 FORMAT(25X,'PERCENT OF HEAT ABSORBED BY THE SOLIDS IN THE CHAR ZONABL2 737	
1E='E15.7/)	ABL2 738
PRINT 610,HREACT	ABL2 739
610 FORMAT(25X,'PERCENT OF HEAT ABSORBED BY REACTION IN THE CHAR ZONE=ABL2 740	
1'E15.7/)	ABL2 741
PRINT586	ABL2 742
586 FORMAT(1H1)	ABL2 743
C	ABL2 744
C-----PRINT OUTPUT PARAMFTERS CORRESPONDING TO JS, GRID SIZE	ABL2 745
C	ABL2 746
IKF=1	ABL2 747
MIKE=5	ABL2 748

LIKE=1	ABL2 749
2602 PRINT 597	ABL2 750
2662 PRINT 5984	ABL2 751
IF(LIKE.GT.1)GO TO 265	ABL2 752
PRINT2650,DELT	ABL2 753
2650 FORMAT(35X,23HTEMPERATURE DROP (OF) =,1X,F20.1/)	ABL2 754
DELP=(P(1)-PL)	ABL2 755
PRINT2651,DELP	ABL2 756
2651 FORMAT(35X,24HPRESSURE DROP (LB/FT2) =,1X,F19.1/)	ABL2 757
PRINT2652,QL	ABL2 758
2652 FORMAT(35X,33HSURFACE HEAT FLUX (BTU/FT2-SEC) =,1X,F10.2/)	ABL2 759
PRINT2653,QR	ABL2 760
2653 FORMAT(35X,32HRADIANT HEAT FLUX BTU/FT2-SEC)=,1X,F11.2/)	ABL2 761
PRINT2654,QA	ABL2 762
2654 FORMAT(35X,35HAERODYNAMIC HEAT FLUX(BTU/FT2-SEC)=,1X,F8.2//)	ABL2 763
265 PRINT2720,(ZX(KK),KK=IKE,MIKE)	ABL2 764
2720 FORMAT(14X,15HCHAR DEPTH (FT),6X,5F13.4)	ABL2 765
PRINT2721,(TP(KK),KK=IKE,MIKE)	ABL2 766
2721 FORMAT(14X,16HTEMPERATURE (OF),5X,5F13.1)	ABL2 767
PRINT2730,(P(KK),KK=IKE,MIKE)	ABL2 768
2730 FORMAT(14X,17HPRESSURE (LB/FT2),4X,5F13.1)	ABL2 769
PRINT2723,(WFLUX(KK),KK=IKE,MIKE)	ABL2 770
2723 FORMAT(14X,21HMASS FLUX(LB/FT2-SEC),5F13.4/)	ABL2 771
PRINT2724	ABL2 772
2724 FORMAT(14X,66H GAS COMPONENT COMPOSITION (	ABL2 773
1MOLE/MOLE GAS)/)	ABL2 774
IF(KEY.GT.1)GOTO2727	ABL2 775
DO 2729 KICK=1,LS	ABL2 776
DO2728LL=1,NS	ABL2 777
YCOMP(LL,KICK)=YI(LL)	ABL2 778
- 2728 CONTINUE	ABL2 779
2727 DO2729LL=1,NS	ABL2 780
YCOMP(LL,1)=YI(LL)	ABL2 781
PRINT 2725,LL,SPCIE1(LL),SPCIE2(LL),(YCOMP(LL,KK),KK=IKE,MIKE)	ABL2 782

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2725 FORMAT(12X,I2,2X,2A3,11X,5E13.4)
2729 CONTINUE
      IF(MIKE.GE.LS)GO TO 2800
      LIKE=LIKE+1
      MIKE=MIKE+5
      IKE=IKE+5
      GO TO 2602
2800 PRINT586
300  STOP
     END
```

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ABL2 783
ABL2 784
ABL2 785
ABL2 786
ABL2 787
ABL2 788
ABL2 789
ABL2 790
ABL2 791
ABL2 792
```

SUBROUTINE CPMIX(T,NN,CPMX)	CPMT	1
C	CPMT	2
C	CPMT	3
C-----THIS SUBROUTINE COMPUTES THE MOLAL HEAT CAPACITY	CPMT	4
C OF A NON-REACTING GAS. IT IS ONLY USE FOR THE	CPMT	5
C FROZEN FLOW CASE.	CPMT	6
COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),AII(30),	CPMT	7
1 RII(30),CII(30),DII(30),EII(30),TLOW(30)	CPMT	8
COMMON/KM/XMOL(30)	CPMT	9
DIMENSION CP(30)	CPMT	10
RR=1.98726	CPMT	11
C	CPMT	12
C CPMX=HEAT CAPCITY(BTU/LB-MOLE-OF)	CPMT	13
C	CPMT	14
C	CPMT	15
C	CPMT	16
C-----CALCULATE THE HEAT CAPACITY OF EACH INDIVIDUAL SPECIE.	CPMT	17
C	CPMT	18
C	CPMT	19
CPMX=0.	CPMT	20
DO 3 I=1,NN	CPMT	21
IF(T.GT.TLOW(I))GOTO1	CPMT	22
CP(I)=(AII(I)+(((EII(I)*T+DII(I))*T+CII(I))*T+RII(I))*T)*RR	CPMT	23
GOTO2	CPMT	24
1 CP(I)=(AI(I)+(((EI(I)*T+DI(I))*T+CI(I))*T+BI(I))*T)*RR	CPMT	25
2 CPMX=CPMX+CP(I)*XMOL(I)	CPMT	26
3 CONTINUE	CPMT	27
RETURN	CPMT	28
END	CPMT	29

C	SUBROUTINE INDPH(TC,CDOV,DCDOV,GASCP,Q,CPV,RHO,TVAR,	INDP	1
C	1 DELTKK,N,DELZ,VR,W,H)	INDP	2
C	DIMENSION DRHODT(5)	INDP	3
C	INDEPTH SUBROUTINE CALCULATES THE PHYSICAL PROPER-	INDP	4
C	TIES FOR THE VIRGIN MATERIAL AND PYROLYSIS GASES.	INDP	5
C	T=TEMPERATURE IN FARENHEIT.	INDP	6
C	IF(N.GT.1)GOTO2	INDP	7
C	DCDOV=.338983E-8	INDP	8
C	READ 1,A,B,C,D,E	INDP	9
C	A THROUGH E ARE CONSTANT FOR THE HEAT CAPACITY OF THE	INDP	10
C	VIRGIN MATERIAL.	INDP	11
C	1 FORMAT(5E12.6)	INDP	12
C	CDOV=THERMAL CONDUCTIVITY OF THE VIRGIN MATERIAL	INDP	13
C	(BTU/(FT-SEC-OF))	INDP	14
C	2 CDOV=1.266102E-5+.338983E-8*TC	INDP	15
C	DCDOV=RATE OF CHANGE OF CDOV WITH TEMPERATURE.	INDP	16
C	T=TC	INDP	17
C	IF(T.GT.750.)GOTO3	INDP	18
C	T2=TC*T	INDP	19
C	T3=TC*T2	INDP	20
C	T4=TC*T3	INDP	21
C	CPV=HEAT CAPACITY OF THE VIRGIN MATERIAL(BTU/LB-OF)	INDP	22
C	CPV=A+B*T+C*T2+D*T3+E*T4	INDP	23
C	3 IF(DELTCK.GT.2.)H=H*2./DELTCK	INDP	24
C	CALL PHMCR(TVAR,DELTCK,QPHNLC,QMICRO,N)	INDP	25
C	IF(TVAR.GE.789.)GOTO200	INDP	26
C		INDP	27
C		INDP	28
C		INDP	29
C		INDP	30
C		INDP	31
C		INDP	32
C		INDP	33
C		INDP	34

CALL NYLON(TVAR,DELTKK,QNYLON)	INDP	35
GOTO210	INDP	36
200 QNYLON=0.	INDP	37
C	INDP	38
210 CALL DNSITY(RHO,TVAR,DELZ,VR,N,DRHODT,W,H)	INDP	39
Q=(QNYLON*DRHODT(1)+QPHNLC*DRHODT(2)+QMICRO*DRHODT(3))*(-1.8)	INDP	40
RETURN	INDP	41
END	INDP	42



	SUBROUTINE CHARPR	CHAR	1
C	CHARPR SUBROUTINE CALCULATES THE EFFECTIVE THERMAL	CHAR	2
C	CONDUCTIVITY AND HEAT CAPACITY OF THE CHAR.	CHAR	3
C		CHAR	4
C	COMMON/KF/CPS,CDO,DCDO,JCHAR,TC	CHAR	5
C		CHAR	6
C	T=TEMPERATURE IN RANKINE	CHAR	7
C	TC=TEMPERATURE IN FARENHEIT	CHAR	8
C	CPS=HEAT CAPACITY OF CHAR(BTU/LB-OF)	CHAR	9
C	CDO=EFFECTIVE THERMAL CONDUCTIVITY(BTU/FT-SEC-OF)	CHAR	10
C	DCDO=RATE OF CHANGE OF CDO WITH TEMPERATURE	CHAR	11
C		CHAR	12
	TC2=TC*TC	CHAR	13
	TC3=TC2*TC	CHAR	14
	IF(TC.GT.2500.)GOTO507	CHAR	15
	T=TC+459.7	CHAR	16
	CPS=0.43+3.6E-5*T-87.2E3/(T*T)	CHAR	17
	IF(TC.LT.1000.)CPS=0.39	CHAR	18
507	CPS=0.52	CHAR	19
	CDO=11.57E-5+5.3E-15*TC3	CHAR	20
	DCDO=15.9E-15*TC2	CHAR	21
	RETURN	CHAR	22
	END	CHAR	23
		CHAR	24

	SUBROUTINE PHMCR(T,DELT,QPHNLC,QMICRO,K6)	PHMC	1
	DIMENSION A(4),B(4),C(4),D(4),E(4),A1(4),B1(4),C1(4),D1(4),E1(4)	PHMC	2
C	THIS SUBROUTINE COMPUTES THE HEAT OF PYROLYSIS OF PHENOLIC,	PHMC	3
C	BASED ON THE DATA OF SYKES AND NELSON(THERMOANALYSIS OF	PHMC	4
C	ABLATION MATERIALS)	PHMC	5
	IF(K6.GT.1)GOTO4	PHMC	6
	NUMBER=4	PHMC	7
	AREA=1350.	PHMC	8
	AREA1=1464.	PHMC	9
C	READ1,NUMBER,AREA,AREA1	PHMC	10
1	FORMAT(I6,2F10.8)	PHMC	11
	DO2I=1,NUMBER	PHMC	12
	READ3,A(I),B(I),C(I),D(I),E(I)	PHMC	13
2	READ3,A1(I),B1(I),C1(I),D1(I),E1(I)	PHMC	14
3	FORMAT(5F12.8)	PHMC	15
4	IF(T.LT.623.)GOTO5	PHMC	16
	IF(T.GT.1073.)GOTO5	PHMC	17
	I=1	PHMC	18
	IF(T.GT.748..AND.T.LT.798.)I=2	PHMC	19
	IF(T.GT.798..AND.T.LT.898.)I=3	PHMC	20
	IF(T.GT.898.)I=4	PHMC	21
	DT=(T-623.)	PHMC	22
	DT2=DT*DT	PHMC	23
	DT3=DT2*DT	PHMC	24
	DT4=DT3*DT	PHMC	25
C	CALCULATE THE HEAT OF PYROLYSIS OF PHENOLIC(QPHNOL)	PHMC	26
	H=A(I)+B(I)*DT+C(I)*DT2+D(I)*DT3+E(I)*DT4	PHMC	27
	QPHNLC=H*DELT*69.312/AREA	PHMC	28
C		PHMC	29
C	69.312=TOTAL HEAT ABSORBED BY THE DECOMPOSITION OF	PHMC	30
C	PHENOLIC IN CAL/GRAM.	PHMC	31
C		PHMC	32
C	CALCULATE THE HEAT OF PYROLYSIS OF PHENOLIC MICRO-	PHMC	33
C	BALLOONS(QMICRO)	PHMC	34

```

      I=1
      IF(T.GT.713..AND.T.LT.798.)I=2
      IF(T.GT.798..AND.T.LT.913.)I=3
      IF(T.GT.913.)I=4
      H=A1(I)+B1(I)*DT+C1(I)*DT2+D1(I)*DT3+E1(I)*DT4
      QMICRO=H*DELT*90.822/AREA1
C      90.822=TOTAL HEAT ABSORBED BY THE DECOMPOSITION OF
C      PHENOLIC MICRO-BALLOONS IN CAL/GRAM.
      RETURN
5     QPHNLC=0.
      QMICRO=0.
6     RETURN
      END

```

```

PHMC  35
PHMC  36
PHMC  37
PHMC  38
PHMC  39
PHMC  40
PHMC  41
PHMC  42
PHMC  43
PHMC  44
PHMC  45
PHMC  46
PHMC  47

```

```

SUBROUTINE NYLON(T,DELT,QNYLON)
C THIS SUBROUTINE COMPUTES THE HEAT OF PYROLYSIS OF NYLON
C BASED ON THE DATA OF SYKES AND NELSON(THERMOANALYSIS OF
C ABLATION MATERIALS)
C
C SLOPE=SLOPE OF LINE OBTAIN FROM SYKES AND NELSON'S DATA.
QNYLON=0.
SLOPE=0.6086957
C
C AREA=1122.
C AREA=AREA UNDER CURVE OF FIGURE-2(DIFFERENTIAL THERMAL
C ANALYSIS) BY SYKES AND NELSON
CONST=150.5738/AREA
IF(T.LT.647.)GOTO4
IF(T.GT.699.)GOTO2
IF(T.GE.689..AND.T.LE.699.)GOTO1
H=SLOPE*(T-647.)
GOTO3
1 H=24.4
GOTO3
2 DH=SLOPE*(T-693.)
H=28.0-DH
IF(T.GE.739.)H=0.
3 QNYLON=DELT*H*CONST
4 RETURN
END

```

```

NYLO 1
NYLO 2
NYLO 3
NYLO 4
NYLO 5
NYLO 6
NYLO 7
NYLO 8
NYLO 9
NYLO 10
NYLO 11
NYLO 12
NYLO 13
NYLO 14
NYLO 15
NYLO 16
NYLO 17
NYLO 18
NYLO 19
NYLO 20
NYLO 21
NYLO 22
NYLO 23
NYLO 24
NYLO 25
NYLO 26

```

SUBROUTINE DENSITY(RHO,T,DELZ,VR,K6,DRHOOT,W,H)	DNSI	1
C	DNSI	2
C	DNSI	3
C-----THIS SUBROUTINE CALCULATES THE DENSITY OF PHENOLIC-NYLON	DNSI	4
C COMPOSITES AS A FUNCTION OF TEMPERATURE--BASED ON DATA	DNSI	5
C OF SYKES AND NELSON(THERMOANALYSIS OF ABLATION MATERIALS)	DNSI	6
C	DNSI	7
C	DNSI	8
C	DNSI	9
COMMON/KK/WTOTAL,RHOI	DNSI	10
REAL*8 RHOT	DNSI	11
C	DNSI	12
DIMENSION RHOI(5),RHOT(5),RHOC(5),A(7),E(7),RATER(7),	DNSI	13
1DRHOOT(5),XN(5,7),FRAC(5),RHOVOL(5)	DNSI	14
DIMENSION MASFRC(5),MASFLX(5),VOLUME(5),VOLFRC(5),DELFLX(5)	DNSI	15
DIMENSION RHOCC(5),DRHO(5)	DNSI	16
INTEGER COMPST	DNSI	17
REAL MASFRC,MASFLX	DNSI	18
C	DNSI	19
C	DNSI	20
IF(K6.GT.1)GOTO7	DNSI	21
C	DNSI	22
C-----READ INPUT	DNSI	23
C	DNSI	24
READ 1,COMPST,NREACT	DNSI	25
1 FORMAT(2I6)	DNSI	26
C	DNSI	27
C	DNSI	28
C COMPST=NUMBER OF COMPOSITE MATERIALS DEGRADING DURING	DNSI	29
C ABLATION.	DNSI	30
C NREACT=NUMBER OF PSEUDO-KINETIC REACTIONS USED TO DES-	DNSI	31
C CRIBE THE DEGRADATION OF THE ABLATIVE COMPOSITES.	DNSI	32
C	DNSI	33
C	DNSI	34

C-----INITIALIZATION OF XN(I,J),WHICH IS THE ORDER OF THE  
C REACTION

C  
C

DO2J=1,NREACT  
DO2I=1,COMPST  
2 XN(I,J)=0.

C  
C  
C  
C  
C

A(J)=FREQUENCY FACTOR(SEC-1)  
E(J)=ENERGY OF ACTIVATION(JOULE/(MOLE))

C  
C  
C  
C  
C  
C  
C  
C  
C  
C  
C  
C

R=8.314  
R=8.314(JOULES/(MOLE-OK))  
RHOI(1)=69.6(NYLON)  
RHOI(2)=80.0(PHENOLIC RESIN)  
RHOI(3)=17.8(PHENOLIC-MICROBALLOONS)  
RHOC(1)=68.6\*0.075=5.145  
RHOC(2)=80.0\*0.541=43.28  
RHOC(3)=17.8\*542=9.6476

C  
C  
C  
C  
C  
C  
C  
C  
C  
C  
C

MASFRC(1)=0.4  
MASFRC(2)=0.25  
MASFRC(3)=0.35

C-----INITIALIZE

C  
C  
C  
C  
C  
C

XN(I,J)=ORDER OF THE KINETIC EXPRESSION.

DNSI 35  
DNSI 36  
DNSI 37  
DNSI 38  
DNSI 39  
DNSI 40  
DNSI 41  
DNSI 42  
DNSI 43  
DNSI 44  
DNSI 45  
DNSI 46  
DNSI 47  
DNSI 48  
DNSI 49  
DNSI 50  
DNSI 51  
DNSI 52  
DNSI 53  
DNSI 54  
DNSI 55  
DNSI 56  
DNSI 57  
DNSI 58  
DNSI 59  
DNSI 60  
DNSI 61  
DNSI 62  
DNSI 63  
DNSI 64  
DNSI 65  
DNSI 66  
DNSI 67  
DNSI 68

DO3J=1,NREACT	DNSI 69
3 READ 4,I,A(J),E(J),XN(I,J)	DNSI 70
4 FORMAT(4X,I6,3E10.8)	DNSI 71
READ 5,(RHOI(I),RHOC(I),MASFRC(I),I=1,COMPST)	DNSI 72
5 FORMAT(3E10.4)	DNSI 73
C	DNSI 74
C	DNSI 75
C RHOI(I)=INITIAL DENSITY OF COMPOSITE I	DNSI 76
C RHOC(I)=RESIDUAL DENSITY OF COMPOSITE I	DNSI 77
C RHOT(I)=DENSITY OF THE COMPOSITE I AT ANY TEMPERATURE	DNSI 78
C	DNSI 79
C	DNSI 80
C-----LET RHOT(I)=RHOI(I) AS INITIAL CONDITION	DNSI 81
C	DNSI 82
C	DNSI 83
DO 6 I=1,COMPST	DNSI 84
RHOCC(I)=RHOC(I)+0.001*RHOC(I)	DNSI 85
MASFLX(I)=0.	DNSI 86
6 RHOT(I)=RHOI(I)	DNSI 87
C	DNSI 88
C	DNSI 89
C-----CALCULATE THE VOLUME FRACTION OF EACH COMPOSITE	DNSI 90
C	DNSI 91
C	DNSI 92
SUMVOL=0.	DNSI 93
DO 60 I=1,COMPST	DNSI 94
VOLUME(I)=MASFRC(I)/RHOT(I)	DNSI 95
60 SUMVOL=SUMVOL+VOLUME(I)	DNSI 96
DO 65 I=1,COMPST	DNSI 97
C	DNSI 98
C VOLFRC(I)=VOLUME FRACTION OF EACH COMPOSITE	DNSI 99
C	DNSI 100
65 VOLFRC(I)=VOLUME(I)/SUMVOL	DNSI 101
C	DNSI 102

C		DNSI 103
C-----	COMPUTE THE DENSITY OF THE COMPOSITE	DNSI 104
C		DNSI 105
C		DNSI 106
C		DNSI 107
C	RHO=DENSITY OF COMPOSITE	DNSI 108
	RHO=1./SUMVOL	DNSI 109
C		DNSI 110
C		DNSI 111
C	RHOII=INITIAL DENSITY OF COMPOSITE	DNSI 112
	RHOII=RHO	DNSI 113
C		DNSI 114
C		DNSI 115
C		DNSI 116
C-----	CALCULATE THE TOTAL MASS FLUX	DNSI 117
C		DNSI 118
C		DNSI 119
C		DNSI 120
C	WTOTAL=TOTAL MASS FLUX(LBS/FT**2-SEC)	DNSI 121
C		DNSI 122
	WTOTAL=RHOII*VR	DNSI 123
	PRINT 66,RHO,WTOTAL	DNSI 124
66	FORMAT(1X,'INITIAL DENSITY OF COMPOSITE(LBS/FT**3)='F10.5,2X,	DNSI 125
1	'WTOTAL(LBS/FT**2-SEC)='E15.7/)	DNSI 126
7	RRR=1000./(R*T)	DNSI 127
	RHOPRV=RHO	DNSI 128
	DO 9 I=1,COMPST	DNSI 129
	SUM=0.	DNSI 130
	DO 8 J=1,NREACT	DNSI 131
	IF(XN(I,J).EQ.0.)GOTO8	DNSI 132
C		DNSI 133
C	RATER(J)=SPECIFIC REACTION VELOCITY	DNSI 134
	IF(RHOT(I).LE.RHOC(I))RHOT(I)=RHOC(I)	DNSI 135
	RATER(J)=-RHOI(I)*((RHOT(I)-RHOC(I))/RHOI(I))**XN(I,J)*A(J)*EXP(-	DNSI 136



1E(J)*RRR)	DNSI 137
SUM=SUM+RATER(J)	DNSI 138
8 CONTINUE	DNSI 139
DRHODT(I)=SUM	DNSI 140
IF(RHOT(I).LE.RHOCC(I))DRHODT(I)=0.	DNSI 141
9 CONTINUE	DNSI 142
C	DNSI 143
C-----CONTROLLING STEP SIZE FOR STABILITY	DNSI 144
C	DNSI 145
TEST=0.	DNSI 146
DO 90 I=1,COMPST	DNSI 147
DRHO(I)=-DELZ*DRHODT(I)/VR	DNSI 148
90 TEST=AMAX1(TEST,DRHO(I))	DNSI 149
IF(TEST.GT.0.1)H=H/2.	DNSI 150
IF(TEST.LT..05)H=H*2	DNSI 151
IF(H.GT.2.08E-4)H=2.08E-4	DNSI 152
C DELZ=STEP SIZE IN FEET	DNSI 153
IF(VR.GE.1.E-2.AND.H.GT.1.E-5)H=1.E-5	DNSI 154
DELZ=H	DNSI 155
RHO=0.	DNSI 156
W=0.	DNSI 157
DO 10 I=1,COMPST	DNSI 158
DEFLX(I)=-DELZ*DRHODT(I)	DNSI 159
C	DNSI 160
C DELFLX(I)=CHANGE IN MASS FLUX DUE TO A CHANGE IN THE	DNSI 161
C DENSITY OF THE COMPOSITES.	DNSI 162
C	DNSI 163
RHOT(I)=RHOT(I)-DEFLX(I)/VR	DNSI 164
RHOVOL(I)=RHOT(I)*VOLFRG(I)	DNSI 165
RHO=RHO+RHOVOL(I)	DNSI 166
C RHO=BULK DENSITY OF THE COMPOSITE	DNSI 167
MASFLX(I)=MASFLX(I)+DEFLX(I)	DNSI 168
10 W=W+MASFLX(I)	DNSI 169
W1=(RHO11-RHO)*VR	DNSI 170

	W=W1	DNSI 171
	DO 100 I=1,COMPST	DNSI 172
100	MASFRC(I)=RHOVOL(I)/RHO	DNSI 173
	PRINT 11,RHO,DELZ,VR,T,W	DNSI 174
11	FORMAT(1X,'RHO(OVERALL DENSITY OF ='F10.4,' DELZ='E10.4,'V='E10.4,	DNSI 175
	1' T='E10.4,' W='E13.5)	DNSI 176
	PRINT 12	DNSI 177
12	FORMAT(8X,'VIRGIN MATERIAL'))	DNSI 178
	DO 14 I=1,COMPST	DNSI 179
	PRINT 13,I,RHOT(I),I,DRHOOT(I),I,DRHO(I),I,MASFRC(I)	DNSI 180
13	FORMAT(1X,'RHOT('I1,')='D12.6,' DROOT('I1,')='E12.6,' DRHO('I1,')=	DNSI 181
	1'E12.6,' MASFRC('I1,')='E12.6)	DNSI 182
14	CONTINUE	DNSI 183
	RETURN	DNSI 184
	END	DNSI 185

C	SUBROUTINE CHARPR CALCULATES THE EFFECTIVE THERMAL	CHAR	1
C	CONDUCTIVITY AND HEAT CAPACITY OF THE CHAR.	CHAR	2
C		CHAR	3
C		CHAR	4
	COMMON/KF/CPS,CDO,DCDO,JCHAR,TC	CHAR	5
C		CHAR	6
C	T=TEMPERATURE IN RANKINE	CHAR	7
C	TC=TEMPERATURE IN FARENHEIT	CHAR	8
C	CPS=HEAT CAPACITY OF CHAR(BTU/LB-OF)	CHAR	9
C	CDO=EFFECTIVE THERMAL CONDUCTIVITY(BTU/FT-SEC-OF)	CHAR	10
C	DCDO=RATE OF CHANGE OF CDO WITH TEMPERATURE	CHAR	11
C		CHAR	12
	TC2=TC*TC	CHAR	13
	TC3=TC2*TC	CHAR	14
	IF(TC.GT.2500.)GOTO507	CHAR	15
	T=TC+459.7	CHAR	16
	CPS=0.43+3.6E-5*T-87.2E3/(T*T)	CHAR	17
	IF(TC.LT.1000.)CPS=0.39	CHAR	18
507	CPS=0.52	CHAR	19
	CDO=11.57E-5+5.3E-15*TC3	CHAR	20
	DCDO=15.9E-15*TC2	CHAR	21
	RETURN	CHAR	22
	END	CHAR	23

SUBROUTINE INTRPL(VAR,X,F,IMAX,SOM)	INTR	1
C	INTR	2
C	INTR	3
C-----THIS PROGRAM PERFORMS LAGRANGIAN INTERPOLATION	INTR	4
C WITH NON-EQUAL STEP SIZE BETWEEN POINTS	INTR	5
C F=DEPENDANT VARIABLE	INTR	6
C X=INDEPENDENT VARIABLE	INTR	7
C VAR=VALUE OF X FOR WHICH CORRESPONDING VALUE OF	INTR	8
C F IS DESIRED BY INTERPOLATION	INTR	9
C IMAX=NUMBER OF POINTS IN ARRAY X OR F	INTR	10
C SOM=VALUE OF INTERPOLATED DEPENDENT VARIABLE	INTR	11
C NPTS=NUMBER OF POINTS USED FOR INTERPOLATION	INTR	12
C	INTR	13
DIMENSION X(100),F(100),XN(300),FN(300)	INTR	14
NPTS=3	INTR	15
607 XUP=1.E30	INTR	16
DO611I=1,IMAX	INTR	17
T=VAR-X(I)	INTR	18
IF(T.GE.0.)GOTO609	INTR	19
608 T=-T	INTR	20
609 IF(T.GE.XUP)GOTO611	INTR	21
610 IP=I	INTR	22
XUP=T	INTR	23
611 CONTINUE	INTR	24
IN=1	INTR	25
NPP=NPTS+1	INTR	26
DO618I=1,NPP	INTR	27
FN(I)=F(IP)	INTR	28
XN(I)=X(IP)	INTR	29
IF(IN.GT.0)GOTO613	INTR	30
612 IQ=IP-I	INTR	31
GOTO615	INTR	32
613 IQ=IP+I	INTR	33
IF(IMAX.GE.IQ)GOTO615	INTR	34

614	IP=IP-1	INTR	35
	GOTO618	INTR	36
615	IF(IQ.GT.0)GOTO617	INTR	37
616	IP=IP+1	INTR	38
	GOTO618	INTR	39
617	IP=IQ	INTR	40
	IN=-IN	INTR	41
618	CONTINUE	INTR	42
	SOM=0.	INTR	43
	FACT=1.	INTR	44
	DO620J=1,NPTS	INTR	45
	SOM=SOM+FACT*FN(I)	INTR	46
	DO619I=J,NPTS	INTR	47
	IQ=I-J+1	INTR	48
619	FN(IQ)=(FN(IQ+1)-FN(IQ))/(XN(I+1)-XN(IQ))	INTR	49
620	FACT=FACT*(VAR-XN(J))	INTR	50
	RETURN	INTR	51
	END	INTR	52

C	SUBROUTINE KINET	KINE	1
C		KINE	2
C		KINE	3
C	-----KINET CALCULATES THE COMPOSITION ,RATE,AND HEAT OF REACTION FOR	KINE	4
C	THE KINETICS MODEL	KINE	5
C		KINE	6
	REAL*8 C,FK,EK,RATER,Z22,H11	KINE	7
C	REAL*8 C,FK,EK,XMULTR,XMULTP	KINE	8
	COMMON/KC/ICODE(30),Y1(30),XFW(30)	KINE	9
	COMMON/KCC/SPCIE1(30),SPCIE2(30),TABLE(300,26),Z,INDPT	KINE	10
	COMMON/KD/RSC(30,30),PSC(30,30),NREX(30,30),NPEX(30,30),	KINE	11
	IAF(30),AEF(30),SF(30),AK(30),BK(30),EKMAX(30),EKMIN(30),NCOEF(30)	KINE	12
	COMMON/KEE/PL,RR,TZERO,EPS,KEY,NC,NS,MM,NQ	KINE	13
	COMMON/KG/ENT(30),RATE(30),T,HEAT1,SUM7	KINE	14
	COMMON/KH/KSP1,NEQ	KINE	15
	COMMON/KI/KN,K7,DTC,HEAT,WEPS,K2,AVGFW,K3,Z2,DELZ,H	KINE	16
	COMMON/KJ/DELTK,TVAR	KINE	17
	COMMON/KQ/Z22	KINE	18
	DIMENSION RATIO(30),RATERR(30)	KINE	19
	DIMENSION TAU(30)	KINE	20
	DIMENSION EKK(30),EK(30)	KINE	21
	DIMENSION FLUXMO(30),FLUXMA(30),C(30),PERCE(30),	KINE	22
1	TEST(30),FK(30),RK(30),RATER(30)	KINE	23
	DIMENSION NSTORE(30),RATE1(30)	KINE	24
	DIMENSION DIFLUX(30)	KINE	25
C		KINE	26
C		KINE	27
C	KEY=3(NONEQUILIBRIUM FLOW)	KINE	28
C	DELZ=FINITE DIFFERENCE STEP SIZE IN CM.	KINE	29
C		KINE	30
	IF(K7.GT.1)GOTO74	KINE	31
	IPRINT=0	KINE	32
C		KINE	33
C	KSP1=TOTAL NUMBER OF CHEMICAL SPECIES(SOLID + GASES)	KINE	34

C	KSP=NUMBER OF GASEOUS SPECIES	KINE	35
C	KSP2=KSP1+1(USED TO IDENTIFY THIRD BODY REACTIONS)	KINE	36
C		KINE	37
C	-----INITIALIZATION OF PARAMENTERS	KINE	38
C		KINE	39
	KPASS=0	KINE	40
	H=1.E-6	KINE	41
	KSP1=NS	KINE	42
	KSP=NC	KINE	43
	KSP2=KSP1+1	KINE	44
	KOS=NS+4	KINE	45
	N=0	KINE	46
	K2=0	KINE	47
	Z22=Z2	KINE	48
	K44=0	KINE	49
C		KINE	50
C	Y1(I)=MOLE FRACTION OF THE CHEMICAL SPECIES	KINE	51
C	KSP2=KSP1+1(USED TO IDENTIFY THIRD BODY REACTION)	KINE	52
C		KINE	53
	DO 83 I=1,KSP2	KINE	54
	DO 83 J=1,KSP2	KINE	55
	RSC(I,J)=0.	KINE	56
	PSC(I,J)=0.	KINE	57
	NREX(I,J)=0	KINE	58
	NPEX(I,J)=0	KINE	59
	83 CONTINUE	KINE	60
C		KINE	61
C	RSC(I,J)=STOICHIOMETRIC COEFFICIENT OF THE REACTANT	KINE	62
C	J IN REACTION I.	KINE	63
C	PSC(I,J)=STOICHIOMETRIC COEFFICIENT OF THE PRODUCTS.	KINE	64
C	NPEX(I,J)=POWER ON THE CONCENTRATION OF THE PRODUCTS.	KINE	65
C	NREX(I,J)=POWER ON THE CONCENTRATION OF THE REACTANTS.	KINE	66
C		KINE	67
C		KINE	68

C-----CONVERT TO KINET UNITS

C

C

ACON4=929.0304/453.59

ACON41=ACON4\*30.48

ACON44=1./ACON4

ACON55=30.48\*\*3/252.

WNEW=WEP5/EP5

W=WNEW

WNEW1=WNEW

C

C

XFW(I)=MOLECULAR WEIGHT OF SPECIE I

C

INPUT SUBROUTINE READS IN THE KINETIC DATA

C

CALL INPUT1

C

K7=2

C

IF K7 IS GREATER THAN 1 CALL INOUT IS BYPASSED

C

P=PL/2160.

C

C

P=PRESSURE(IN ATMOSPHERES)

C

R=82.06

C

C

R AND RR ARE UNIVERSAL GAS CONSTANTS IN DIFFERENT UNITS.

C

C-----CALCULATE INITIAL AVERAGE MOLECULAR WEIGHT

C

SUM=0.

DO1J=1,KSP

1 SUM=SUM+XFW(J)\*Y1(J)

AVGFW=SUM

ACON1=W/AVGFW\*ACON44

KINE 69

KINE 70

KINE 71

KINE 72

KINF 73

KINE 74

KINE 75

KINE 76

KINE 77

KINE 78

KINE 79

KINE 80

KINE 81

KINE 82

KINE 83

KINE 84

KINE 85

KINE 86

KINE 87

KINE 88

KINE 89

KINE 90

KINE 91

KINE 92

KINE 93

KINE 94

KINE 95

KINE 96

KINE 97

KINE 98

KINE 99

KINE 100

KINE 101

KINE 102



C	ACON1=TOTAL MOLAL FLUX IN GRAM-MOLES/(CM2-SEC)	KINE 103
C		KINE 104
C		KINE 105
C		KINE 106
C	-----CALCULATE INITIAL MOLAL FLUX(FLUXMO--GM-MOLES/CM2-SEC)	KINE 107
C		KINE 108
C		KINE 109
	DO2J=1,KSP1	KINE 110
	FLUXMO(J)=ACON1*Y1(J)	KINE 111
C		KINE 112
C		KINE 113
C	-----CALCULATE INITIAL MASS FLUX(FLUXMA)	KINE 114
C		KINE 115
C		KINE 116
2	FLUXMA(J)=FLUXMO(J)*XFW(J)	KINE 117
	WNEW2=W	KINE 118
	TPREV=TVAR-5.	KINE 119
C		KINE 120
C	-----CONVERT STEP SIZE TO CENTIMETERS	KINE 121
C		KINE 122
74	DELZZ=DELZ*30.48	KINE 123
	T=TVAR	KINE 124
	XDELTT=TVAR-TPREV	KINE 125
	SUM1=0.	KINE 126
	RRR=1000./(RR*T)	KINE 127
	ACON9=R*T/P	KINE 128
	DO5J=1,KSP	KINE 129
5	SUM1=SUM1+FLUXMO(J)*ACON9	KINE 130
C		KINE 131
C		KINE 132
C	-----CALCULATE THE CONCENTRATION C(J) OF THE SPECIES(GM-MOLES/CM3)	KINE 133
C		KINE 134
C		KINE 135
	SUM=0.	KINE 136

DO6J=1,KSP	KINE 137
C(J)=FLUXMO(J)/SUM1	KINE 138
6 SUM=SUM+C(J)	KINE 139
C(KSP1)=SUM*Y1(KSP1)	KINE 140
C(KSP2)=SUM	KINE 141
C	KINE 142
C C(KSP2)=CONCENTRATION USE FOR A THIRD BODY REACTION	KINE 143
C	KINE 144
C	KINE 145
C-----CALCULATE FK AND RK WHICH ARE THE FOWARD	KINE 146
C AND REVERSE REACTION RATE CONSTANTS.	KINE 147
C	KINE 148
C	KINE 149
RT=R*T	KINE 150
C EK=EQUILIBIRUM CONSTANT	KINE 151
DO7I=1,NEQ	KINE 152
IF(SF(I).EQ.0.)GOTO900	KINE 153
FK(I)=AF(I)*T**(-SF(I))*EXP(-AEF(I)*RRR)	KINE 154
GOTO902	KINE 155
900 FK(I)=AF(I)*EXP(-AEF(I)*RRR)	KINE 156
902 A1=AK(I)	KINE 157
A2=BK(I)	KINE 158
EKK(I)=EXP(A1+A2/T)	KINE 159
X12=EKMAX(I)	KINE 160
IF(EKK(I).GT.EKMAX(I))EKK(I)=EKMAX(I)	KINE 161
IF(EKK(I).LT.EKMIN(I))EKK(I)=EKMIN(I)	KINE 162
EK(I)=EKK(I)/(RT*NCDEF(I))	KINE 163
RK(I)=FK(I)/EK(I)	KINE 164
7 CONTINUE	KINE 165
C	KINE 166
C	KINE 167
C-----CALCULATION OF REACTION RATE OF SPECIE(J)	KINE 168
C	KINE 169
C	KINE 170

C

RATER(1)=FK(1)*(C(3)-C(1)*C(8)/EK(1))	KINE 171
RATER(2)=FK(2)*(C(3)-C(2)*C(9)/EK(2))	KINE 172
RATER(3)=FK(3)*(C(2)*C(2)-C(4)/EK(3))	KINE 173
RATER(4)=FK(4)*(C(4)-C(5)*C(8)/EK(4))	KINE 174
RATER(5)=FK(5)*(C(5)-C(6)*C(8)/EK(5))	KINE 175
RATER(6)=FK(6)*(C(6)-C(8)/EK(6))	KINE 176
RATER(7)=FK(7)*(C(6)-C(7)*C(9)/EK(7))	KINE 177
RATER(8)=FK(8)*(C(16)-C(14)*C(8)/EK(8))	KINE 178
RATER(9)=FK(9)*(C(15)-C(14)*C(14)/EK(9))	KINE 179
RATER(10)=FK(10)*(C(8)-C(9)*C(9)/EK(10))	KINE 180
RATER(11)=FK(11)*(C(16)-C(17)*C(9)/EK(11))	KINE 181
RATER(12)=FK(12)*(C(9)*C(15)-C(14)*C(17)/EK(12))	KINE 182
RATER(13)=FK(13)*(C(15)-C(14)*C(18)/EK(13))	KINE 183
RATER(14)=FK(14)*(C(11)*C(8)-C(12)*C(16)/EK(14))	KINE 184
RATER(15)=FK(15)*(C(12)-C(6)*C(6)*C(6)/EK(15))	KINE 185
DO 121 I=1,KSP1	KINE 186
XJ=RATER(I)	KINE 187
IF(XJ.LT.0.)RATER(I)=0.	KINE 188
121 CONTINUE	KINE 189
RATE(1)=RATER(1)	KINE 190
RATE(2)=RATER(2)-2.*RATER(3)	KINE 191
RATE(3)=-RATER(1)-RATER(2)	KINE 192
RATE(4)=RATER(3)-RATER(4)	KINE 193
RATE(5)=RATER(4)-RATER(5)	KINE 194
RATE(6)=RATER(5)-RATER(6)-RATER(7)+3.*RATER(15)	KINE 195
RATE(7)=RATER(7)	KINE 196
RATE(8)=RATER(1)+RATER(4)+RATER(5)+RATER(6)+RATER(8)-RATER(10)-	KINE 197
1 RATER(14)	KINE 198
RATE(9)=RATER(2)+RATER(7)+2.*RATER(10)+RATER(11)-RATER(12)	KINE 199
RATE(10)=0.	KINE 200
RATE(11)=-RATER(14)	KINE 201
RATE(12)=RATER(14)-RATER(15)	KINE 202
RATE(13)=0.	KINE 203
	KINE 204

RATE(14)=RATER(8)+2.*RATER(9)+RATER(12)+RATER(13)	KINE 205
RATE(15)=-RATER(9)-RATER(12)-RATER(13)	KINE 206
RATE(16)=-RATER(8)-RATER(11)+RATER(14)	KINE 207
RATE(17)=RATER(11)+RATER(12)	KINE 208
RATE(18)=RATER(13)	KINE 209
RATE(19)=RATER(6)*2.-RATER(8)-RATER(9)	KINE 210
C RATE(J)= REACTION RATE(GRAM-M/LES/(CM3-SEC)) FOR SPECIE J.	KINE 211
C	KINE 212
TPREV=TVAR	KINE 213
K44=K44+1	KINE 214
DSUM=0.	KINF 215
DSUMM=0.	KINE 216
TESS=0.	KINE 217
DO 130 I=1,KSP1	KINE 218
DLFLUX(I)=RATE(I)*XFW(I)*DELZZ	KINE 219
RATIO=DLFLUX(I)/FLUXMA(I)	KINE 220
RATIO(I)=RATIO	KINE 221
IF(RATIO.GE.0.)GOTO129	KINE 222
RATO=ABS(RATIO)	KINE 223
IF(RATO.GT.0.1)KPASS=1	KINE 224
129 ADFLUX=ABS(DLFLUX(I))	KINE 225
TESS=AMAX1(TESS,ADFLUX)	KINE 226
DSUM=DSUM+DLFLUX(I)	KINE 227
IF(I.GT.KSP)GOTO130	KINE 228
DSUMM=DSUM	KINE 229
130 CONTINUE	KINF 230
C	KINE 231
C-----CHECK STEP SIZE FOR STABILITY	KINE 232
C	KINE 233
IF(KPASS.EQ.1)H=H/4.	KINE 234
IF(H.GT.1.08E-4)H=1.08E-4	KINE 235
IF(RATO.LT.0.010)H=H*2	KINF 236
IF(H.LT.2.5E-7)H=2.5E-7	KINF 237
DELZZ=H*30.48	KINE 238

DO 13 J=1,KSP1	KINE 239
TEST(J)=FLUXMA(J)	KINE 240
FLUXMA(J)=FLUXMA(J)+RATE(J)*DELZZ*XFW(J)	KINE 241
IF(FLUXMA(J).GE.0.)GOTO13	KINE 242
FLUXMA(J)=1.E-40	KINE 243
13 CONTINUE	KINE 244
KPASS=0	KINE 245
WNEW1=WNEW1-RATE(KSP1)*DELZZ*XFW(KSP1)*ACON4	KINE 246
WNEW=WNEW1	KINE 247
WEPS=WNEW*EPS	KINE 248
WNEW2=0.	KINE 249
SUM3=0.	KINE 250
132 DO 19 J=1,KSP1	KINE 251
FLUXMO(J)=FLUXMA(J)/XFW(J)	KINE 252
IF(J.GT.KSP)GOTO19	KINE 253
SUM3=SUM3+FLUXMO(J)	KINE 254
WNEW2=WNEW2+FLUXMA(J)	KINE 255
19 CONTINUE	KINE 256
WNEW2=WNEW2*ACON4	KINE 257
WNEW22=WNEW2	KINE 258
DO14J=1,KSP1	KINE 259
Y1(J)=FLUXMO(J)/SUM3	KINE 260
14 PERCE(J)=Y1(J)*100.	KINE 261
SUM=0.	KINE 262
DO 111 I=1,KSP	KINE 263
SUM=SUM+XFW(I)*Y1(I)	KINE 264
111 CONTINUE	KINE 265
AVGFW=SUM	KINE 266
RHO=ACON41/ACON9*AVGFW	KINE 267
VEL=WNEW/RHO	KINE 268
C	KINE 269
C-----CONVERT THE UNITS OF THE HEAT OF REACTION	KINE 270
C TERM TO THOSE COMPATIBLE WITH GROUP	KINE 271
C	KINE 272

C	CALL THERM2	KINF 273
C		KINE 274
C	HEAT=RATE OF HEAT ABSORBED OR RELEASE BY CHEMICAL	KINE 275
C	REACTIONS(BTU/FT**3-SEC).	KINE 276
C		KINE 277
	HEAT=HEAT1*ACON55	KINE 278
	HEAT3=HEAT/DTC	KINE 279
	H11=H	KINE 280
	Z22=Z22+H11	KINE 281
	IF(Z2.LE.Z22)GOTO37	KINF 282
	RETURN	KINE 283
37	K2=K2+1	KINE 284
	IF(K2.GE.299)K2=299	KINE 285
	DO17 I=5,KOS	KINE 286
	TABLE(K2,I)=Y1(I-4)	KINE 287
17	CONTINUE	KINE 288
	TABLE(K2,1)=T	KINE 289
	TABLE(K2,2)=HEAT	KINE 290
	TABLE(K2,3)=AVGFW	KINE 291
	TABLE(K2,4)=WNEW	KINE 292
	PRINT 94, WNEW,WNEW2,DELZ,XDELTT	KINF 293
	PRINT 776	KINE 294
776	FORMAT(1H1, //11X, 'HEAT OF FORMATION', 3X, 'MOLE FRACTION',	KINE 295
1	5X, 'RATE(I)', 9X, 'RATER(I)', 8X, 'FLUXMA(I)' ///)	KINE 296
	DO 779 I=1, KSP1	KINE 297
	PRINT 777, SPCIE1(I), SPCIE2(I), ENT(I), Y1(I), RATE(I),	KINE 298
1	RATER(I), FLUXMA(I), DLFLUX(I), RATIO(I)	KINE 299
777	FORMAT(6X, 2A3, 7E16.7)	KINE 300
779	CONTINUE	KINE 301
	PRINT 780	KINE 302
780	FORMAT(1H0)	KINE 303
	PRINT 781, Z, H, K2, K3, K44, Z22, DSUM, DSUMM	KINF 304
781	FORMAT(6X, 'Z='1E12.6, 3X, 'H='E12.6, 3X, 'K2='I3, ' K3='I8, 1X,	KINE 305
		KINE 306

1'K44='I6,' Z22='D18.9,2E16.7)	KINE 307
PRINT 6022,T	KINE 308
6022 FORMAT(7X,18HTEMPERATURE IN OK=,1F10.3)	KINE 309
TF=T*1.8-460.0	KINE 310
PRINT 6023,TF	KINE 311
6023 FORMAT(7X,18HTEMPERATURE IN OF=,1F10.3)	KINE 312
6024 FORMAT(7X,40HHEAT ABSORBED BY REACTIONS(BTU/FT2-SEC)=,1F14.5)	KINE 313
PRINT 6024,HEAT3	KINE 314
PRINT 6025,WNEW	KINE 315
6025 FORMAT(7X,18HOVERALL MASS FLUX=,E14.7)	KINE 316
PRINT 6026,AVGFW	KINE 317
6026 FORMAT(7X,32HAVERAGE MOLECULAR WEIGHT OF GAS=,1F10.3///)	KINE 318
PRINT 6032,SUM7	KINE 319
6032 FORMAT(//10X,36HENTHALPY OF THE REACTING GAS SYSTEM=,1E16.8)	KINE 320
94 FORMAT(1X,5E20.8)	KINE 321
PRINT 95,VEL,RHO	KINE 322
95 FORMAT(1X,'VEL(FT/SEC)='E15.7,' RHO(LBS/FT3)='E15.7/)	KINE 323
RETURN	KINE 324
END	KINE 325

<pre> C C C-----THERMO SUBROUTINE CALCULATES THE HEAT OF REACTION OF C THE MIXTURE,THE HEAT OF FORMATION OF EACH INDIVIDUAL C CHEMICAL SPECIE, AND THE HEAT CAPACITY OF THE MIXTURE C C COMMON/KA/S1(6),S2(6),S3(6),S4(6),S5(6),A11(6),A22(6), 1 A33(6),A44(6),A55(6),FI(30),FII(30),GI(30), 2 GII(30),AA(30,6),S6(6),A66(6),JCODE(6),CPMX COMMON/KB/AI(30),BI(30),CI(30),DI(30),EI(30),AII(30), 1 BII(30),CII(30),DII(30),EII(30),TLOW(30) COMMON/KC/ICODE(30),Y(30),FW(30) COMMON/KG/ENT(30),RATE(30),T,HEAT1,SUM7 COMMON/KEE/PL,RR,TZERO,EPS,KEY,NC,NS,MM,NQ DIMENSION CPDT1(6),ENT1(30),CP(30)  C C TEMPERATURE IN OK. C T1=T T2=T1*T T3=T2*T T4=T3*T T5=T4*T A1=T A2=T2/2. A3=T3/3. A4=T4/4. A5=T5/5. CPMX=0. SUM7=0. HEAT1=0. DO 78 I=1,NQ </pre>	<pre> THER 1 THER 2 THER 3 THER 4 THER 5 THER 6 THER 7 THER 8 THER 9 THER 10 THER 11 THER 12 THER 13 THER 14 THER 15 THER 16 THER 17 THER 18 THER 19 THER 20 THER 21 THER 22 THER 23 THER 24 THER 25 THER 26 THER 27 THER 28 THER 29 THER 30 THER 31 THER 32 THER 33 THER 34 </pre>
---	---



IF(T.LT.TLOW(I))GOTO6207	35	35
C	36	36
TLOW(I)=MINIMUM TEMPERATURE AT WHICH THE HIGH	37	37
TEMPERATURE FIT CAN BE USED.	38	38
C	39	39
ENT1=SENSIBLE ENTHALPY+CHEMICAL POTENTIAL	40	40
C	41	41
ENT1(I)=(AI(I)*A1+BI(I)*A2+CI(I)*A3+DI(I)*A4+EI(I)*A5	42	42
1+FI(I))*RR	43	43
C	44	44
CP=HEAT CAPACITY	45	45
CP(I)=(AI(I)+BI(I)*T1+CI(I)*T2+DI(I)*T3+EI(I)*T4)*RR	46	46
IF(I.GT.1)GOTO6291	47	47
C	48	48
C	49	49
C-----CALCULATE THE SENSIBLE ENTHALPY OF THE CONSTITUENT	50	50
C	51	51
C	52	52
C	53	53
DO296J=1,MM	54	54
CPDT1(J)=(S1(J)*A1+S2(J)*A2+S3(J)*A3+S4(J)*A4+S5(J)*A5	55	55
1 +S6(J))*RR	56	56
296 CONTINUE	57	57
GOTO6291	58	58
C	59	59
6207 ENT1(I)=(AII(I)*A1+BII(I)*A2+CII(I)*A3+DII(I)*A4+EII(I)*A5	60	60
1+FII(I))*RR	61	61
CP(I)=(AII(I)+BII(I)*T+CII(I)*T2+DII(I)*T3+EII(I)*T4)*RR	62	62
IF(I.GT.1)GOTO6291	63	63
DO297J=1,MM	64	64
CPDT1(J)=(A11(J)*A1+A22(J)*A2+A33(J)*A3+A44(J)*A4	65	65
1 +A55(J)*A5+A66(J))*RR	66	66
297 CONTINUE	67	67
C	68	68
C		

C	JCODE(J)=0 THE REFERENCE ELEMENT IS IN THE GAS STATE.	THER	69
C	JCODE(J)=1 THE REFERENCE ELEMENT IS IN THE SOLID STATE.	THER	70
C		THER	71
C	-----RSUM IS THE SUM OF THE SENSIBLE ENTHALPY OF THE CONSTI-	THER	72
C	TUENT ELEMENTS OF THE ITH SPECIE AT TEMPERATURE T(OK),	THER	73
C	WITH RESPECT TO THE STANDARD STATE(P=1 ATM AND T=298 )	THER	74
C		THER	75
C		THER	76
	6291 RSUM=0.	THER	77
	DO398J=1,MM	THER	78
	IF(JCODE(J).EQ.1)GOTO393	THER	79
	RSUM=RSUM+0.5*AA(I,J)*CPDT1(J)	THER	80
	GOTO398	THER	81
	393 RSUM=RSUM+AA(I,J)*CPDT1(J)	THER	82
	398 CONTINUE	THER	83
C		THER	84
C	-----CALCULATE THE HEAT OF FORMATION ENT(I) FOR EACH SPECIE .	THER	85
C		THER	86
	ENT(I)=ENT1(I)-RSUM	THER	87
	IF(ABS(ENT(I)).LT.3.)ENT(I)=0.	THER	88
C		THER	89
C	-----CALCULATE HEAT1,WHICH IS THE HEAT ABSORBED BY THE CHEMICAL	THER	90
C	REACTIONS(CALORIES/GM-MOLE)	THER	91
C		THER	92
	IF(I.GT.NC)GOTO8005	THER	93
	HEAT1=HEAT1+RATE(I)*EPS*ENT(I)	THER	94
	GO TO 787	THER	95
	8005 HEAT1=HEAT1+RATE(I)*(1.-EPS)*ENT(I)	THER	96
	GO TO 78	THER	97
	787 SUM7=SUM7+Y(I)*ENT1(I)	THER	98
	CPMX=CPMX+CP(I)*Y(I)	THER	99
	78 CONTINUE	THER	100
	RETURN	THER	101
	END	THER	102

	SUBROUTINE INPUT1	INPU	1
	COMMON/KD/RSC(30,30),PSC(30,30),NREX(30,30),NPEX(30,30),	INPU	2
	1AF(30),AEF(30),SF(30),AK(30),BK(30),EKMAX(30),EKMIN(30),NCOEF(30)	INPU	3
	COMMON/KH/KSP1,NEQ	INPU	4
	DIMENSION EQN(30,30)	INPU	5
C		INPU	6
C		INPU	7
C		INPU	8
C	RSC(I,J)=STOICHIOMETRIC COEFFICIENT OF REACTANT I IN REACTION J.	INPU	9
C	PSC(I,J)=STOICHIOMETRIC COEFFICIENT OF PRODUCT I IN REACTION J.	INPU	10
C	NREX(I,J)=POWER ON CONCENTRATION OF REACTANT I.	INPU	11
C	NPEX(I,J)=POWER ON CONCENTRATION OF PRODUCT I.	INPU	12
C	AF(J)=FREQUENCY FACTOR OF FORWARD REACTION.	INPU	13
C	SF(J)=POWER DEPENDENCE ON TEMPERATURE FOR FORWARD REACTION.	INPU	14
C	AEF(J)=ACTIVATION ENERGY OF FORWARD REACTION.	INPU	15
C	EQN=ALPHA-NUMERIC STORAGE OF TITLE OF CHEMICAL REACTION.	INPU	16
C	AK AND BK=EMPIRICAL CONSTANT FOR EQUILIBRIUM CONST. FIT.	INPU	17
C	AK AND BK ARE EMPIRICAL CONSTANTS FOR THE EQUILIBRIUM CONSTANT FIT	INPU	18
C	EKMAX AND EKMIN ARE THE MAX. AND MIN. VALUE OF THE EQUILIBRIUM	INPU	19
C	CONSTANTS. THESE VALUES ARE USED TO AVOID EXTREME CASES. THESE	INPU	20
C	ARE WHEN THE CONVERSION IS CLOSE TO ONE, OR CLOSE TO ZERO.	INPU	21
C	COEF(J)=SUM COEF. OF OF CONCENTRATION OF PROD. MINUS REACT.	INPU	22
C	KSP1=TOTAL NUMBER OF GASES AND SOLIDS SPECIES.	INPU	23
C	NEQ=NUMBER OF CHEMICAL REACTIONS.	INPU	24
C		INPU	25
C		INPU	26
C		INPU	27
C	READ INPUT	INPU	28
C		INPU	29
C		INPU	30
10	CONTINUE	INPU	31
	READ 1,NEQ	INPU	32
1	FORMAT(I2)	INPU	33
	PRINT 12	INPU	34

	DO 6 J=1,NEQ	INPU 35
	READ 7,(EQN(J,K),K=1,19)	INPU 36
7	FORMAT(19A4)	INPU 37
	PRINT 13,(EQN(J,I),I=1,19)	INPU 38
	READ 2,I,RSC(J,I),I,RSC(J,I),I,RSC(J,I),I,PSC(J,I),I,PSC(J,I),	INPU 39
1	I,PSC(J,I)	INPU 40
	READ 3,I,NREX(J,I),I,NREX(J,I),I,NREX(J,I),I,NPEX(J,I),	INPU 41
1	I,NPEX(J,I),I,NPEX(J,I)	INPU 42
	READ 4,AF(J),SF(J),AEF(J)	INPU 43
	READ 5,AK(J),BK(J),EKMAX(J),EKMIN(J),NCOEF(J)	INPU 44
2	FORMAT(6(I3,F3.0))	INPU 45
3	FORMAT(12I3)	INPU 46
4	FORMAT(E8.0,2X,2F10.1)	INPU 47
5	FORMAT(4E15.7,I5)	INPU 48
6	CONTINUE	INPU 49
11	CONTINUE	INPU 50
	PRINT 12	INPU 51
12	FORMAT(1H1)	INPU 52
13	FORMAT(1X,19A4/)	INPU 53
	RETURN	INPU 54
	END	INPU 55

SUBROUTINE INTRPL(VAR,X,F,IMAX,SOM)	INTR	1
DIMENSION X(1),F(1),XN(100),FN(100)	INTR	2
C	INTR	3
C*****	INTR	4
C* THIS PROGRAM PERFORMS LAGRAGIAN INTERPOLATION *	INTR	5
C* WITH UNEQUAL STEP SIZE BETWEEN POINTS. *	INTR	6
C*****	INTR	7
C	INTR	8
C F=DEPENDENT VARIABLE	INTR	9
C X=INDEPENDENT VARIABLE	INTR	10
C VAR=VALUE OF X FOR WHICH CORRESPONDING VALUE OF	INTR	11
C F IS DESIRED BY INTERPOLATION	INTR	12
C IMAX=NUMBER OF POINTS IN ARRAY X OR F.(MAX OF 100 )	INTR	13
C SOM=VALUE OF INTERPOLATED DEPENDENT VARIABLE	INTR	14
C NPTS=NUMBER OF POINTS USED FOR INTERPOLATION	INTR	15
NPTS=3	INTR	16
607 XUP=1.E30	INTR	17
DO 611 I=1,IMAX	INTR	18
T=VAR-X(I)	INTR	19
IF(T.GE.0.)GO TO 609	INTR	20
608 T=-T	INTR	21
609 IF (T .GE. XUP) GO TO 611	INTR	22
610 IP=I	INTR	23
XUP=T	INTR	24
611 CONTINUE	INTR	25
IN=1	INTR	26
NPP=NPTS+1	INTR	27
DO 618 I=1,NPP	INTR	28
FN(I)=F(IP)	INTR	29
XN(I)=X(IP)	INTR	30
IF(IN .GT. 0.) GO TO 613	INTR	31
612 IQ=IP-I	INTR	32
GO TO 615	INTR	33
613 IQ=IP+I	INTR	34

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        IF (IMAX .GE. IO) GO TO 615
614  IP=IP-1
      GO TO 618
615  IF (IQ .GT. 0 ) GO TO 617
616  IP=IP+1
      GO TO 618
617  IP=IQ
      IN =-IN
618  CONTINUE
      SOM=0.
      FACT=1.
      DO 620 J=1,NPTS
        SOM=SOM+FACT*FN(I)
        DO 619 I=J,NPTS
          IQ=I-J+1
619  FN(IQ)=(FN(IQ+1)-FN(IQ)/XN(I+1)-XN(IQ))
620  FACT=FACT*(VAR-XN(J))
      RETURN
      END

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INTR 35
INTR 36
INTR 37
INTR 38
INTR 39
INTR 40
INTR 41
INTR 42
INTR 43
INTR 44
INTR 45
INTR 46
INTR 47
INTR 48
INTR 49
INTR 50
INTR 51
INTR 52
INTR 53

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## ABLATIN2 ANALYSIS NOMENCLATURE

### MAIN:

AA(I,J): Formula number. Gives the gram atoms of element J in species I.

AI...GI: These are the seven empirical constants for the high temperature fit ( $1000^{\circ}\text{K}$ - $6000^{\circ}\text{K}$ ) for the free energy functions. The first five constants (AI through EI) are used in the heat capacity fit.

AII...GII: These are the seven empirical constants for the low temperature fit ( $300^{\circ}\text{K}$ - $1000^{\circ}\text{K}$ ) for the free energy function.

A11...A66: These are the six empirical constants for the enthalpy fit of the constituent elements ( $300^{\circ}\text{K}$ - $1000^{\circ}\text{K}$ ).

ALPHA: Viscous coefficient in Darcy's equation ( $\text{FT}^{-1}$ ).

AVGFW: Average molecular weight of the gas mixture.

BETA: Inertial coefficient in Darcy's equations ( $1/\text{FT}^2$ ).

CDO: Thermal conductivity of the char ( $\text{BTU}/\text{FT}\text{-sec-}^{\circ}\text{F}$ ).

CDOV: Thermal conductivity of the virgin material, ( $\text{BTU}/\text{FT}\text{-sec-}^{\circ}\text{F}$ ).

CPB1: Total rate of heat absorbed by the gases in the char zone. ( $\text{BTU}/\text{FT}^2\text{sec}$ ).

CPB2: Total rate of heat absorbed by the solids in the char zone. ( $\text{BTU}/\text{FT}^2\text{sec}$ ).

CPS: Heat capacity of the char (BTU/lb-°F).

CPV: Heat capacity of the virgin material (BTU/lb-°F).

DCDO: Rate of change of the thermal conductivity of the char with temperature. (BTU/FT-sec-°F<sup>2</sup>).

DCDOV: Rate of change of the thermal conductivity of the virgin material with temperature. (BTU/FT-sec-°F<sup>2</sup>).

DELTF: Differential change in temperature in °F for an increment of distance H.

DELTK: Differential change in temperature in °K for an increment of distance H.

DELTP: Pressure drop across the char. (lbs./ft<sup>2</sup>).

DELZ: Increment of distance (in feet).

DISTAN: Char thickness in feet.

DT: Temperature gradient (°F/FT).

DTC: Temperature gradient in the char (°F/FT).

DTCC: Temperature gradient in double precision arithmetic in the char (°F/FT).

DTCI: Temperature gradient in the virgin material (°F/FT).

EK: Potential parameter /Boltzman constant.

EMIS: Char emissivity.

EPS: Porosity of the char (FT<sup>2</sup> voids/FT<sup>2</sup> total).

FW(I): Molecular weight of species I.

GASCP: Is the heat capacity of the gas mixture in (BTU/lb-°F).

GROUP: This is the bracketted term of Equation (3-36). (1/FT).



H: Runge-Kutta step size (in feet).

H11: Runge-Kutta step size in double precision arithmetic (in feet).

HCHAR: Percent of total heat absorbed in the char zone.

HDECOM: Percent of total heat absorbed in the decomposition zone.

HGAS: Percent of heat absorbed by the gas in the char zone.

HI: Initial value of Runge-Kutta step (in feet).

HREACT: Percent of heat absorbed by the reactions in the char zone.

HSOLID: Percent of heat absorbed in the solids in the char zone.

ICODE(I): Is a code to identify whether a species is a gas or a solid. If ICODE is zero, the species is a gas. If ICODE is one, the species is a solid.

IMAX: Number of data points for EK.

ITEMP: Total number of temperature points stored in temperature profile.

JCODE(J): Is a code used to determine whether the reference state of the constituent element J is in the gas or in the solid state.

JS: Total number of slices in which the char is divided for the solution of the momentum equation.

K1: Is a counter for the number of temperature points stored during the solution of the energy equation.

MM: Is the number of elements.

NC: Number of gas species read in.

NDATA: Number of collision integral points tabulated versus XTKE.

NN: Number of gas species in the system.

NN5: Is the total number of variables stored in TABLE (I,J).

NNS: Is the number of solid species in the system.

NQ: Is the total number of gas and solid species in the system.

NS: Is the total number of gas and solid species read in.

OMGA: Interpolated value of XTKE.

P: Pressure in  $\text{lbs/ft}^2$ .

PL: Pressure at the front surface of the char ( $\text{lbs/ft}^2$ ).

Q: Is the rate of heat absorbed in the decomposition zone in  $(\text{BTU/ft}^3\text{sec})$ .

Q2: It equals  $Q/\text{DTC}$   $(\text{BTU/FT}^2\text{-sec-}^\circ\text{F})$ .

QA: Aerodynamic heating rate  $(\text{BTU/FT}^2\text{-sec})$ . Equals  $QL+QR$ .

QCZ: Heat flux in the char zone  $(\text{BTU/ft}^2\text{-sec})$ .

QCZI: Heat flux in the decomposition zone  $(\text{BTU/ft}^2\text{sec})$ .

QL: Is the total heat flux at the surface  $(\text{BTU/ft}^2\text{sec})$ .

QR: Is the rate of re-radiation from the surface of the char  $(\text{BTU/ft}^2\text{-sec})$ .

REAC1: Is the total rate of heat absorbed by the che-

mical reactions. (BTU/ft<sup>2</sup>-sec).

REAC2: Heat absorbed by the chemical reactions (BTU/ft<sup>2</sup>-sec).

REACT: Equals REAC2/DTC (BTU/ft<sup>2</sup>-sec-°F).

RHO: Bulk density of the virgin material (lbs/ft<sup>3</sup>).

ROCHAR: Bulk density of the char material (lbs/ft<sup>3</sup>).

RR: Gas constant: 1.98726 (BTU/lb-mole °R).

S1...S6: These are six empirical constants for the enthalpy fit of the constituent elements (1000°K-6000°K).

SIG: Collision diameter (Angstroms).

SIGMA: Stephan-Boltzman constant ( $4.81 \times 10^{-13}$  BTU/ft<sup>2</sup>-sec-°F<sup>4</sup>).

TL(K1): Variable in which the temperature profile is stored versus distance Z. K1 is a counter.

TC: Temperature in °F.

TCHAR: Temperature at which all the virgin material has degraded to gas and char (°K).

TFMAX: Maximum specified temperature of the front surface of the char (°F).

THICK: Is the thickness of the char zone, in inches.

THICK1: Is the thickness of the decomposition zone in inches.

TK: Interpolated value of the temperature (in°K) at a distance Z in the char.

TL: Front surface temperature of the char (°F) when the temperature profile has been defined.

TLOW(I): Maximum temperature of low temperature fit

for species I. ( $^{\circ}\text{K}$ )

TO: Initial temperature (in  $^{\circ}\text{F}$ ) at  $Z=0$ .

TPREV: Temperature (in  $^{\circ}\text{F}$ ) at the previous step.

TTTT: This is the temperature (in  $^{\circ}\text{F}$ ) in double precision arithmetic. A provision has been made in the program that if the step size is less than  $8. \times 10^{-9}$  ft., the Runge-Kutta analysis is calculated in double precision arithmetic to reduce round-off error.

TVAR: Temperature in  $^{\circ}\text{K}$ .

TVIS: Interpolated value of the temperature profile (in  $^{\circ}\text{F}$ ) at a distance  $Z$  along the char.

VISCOS: Viscosity of the gas (in centipoise).

VR: Surface recession velocity (ft/sec).

W: Mass flux based on the total area (lbs/ft<sup>2</sup>-sec).

WI: Mass flux of the gases entering the char based on the total area (lbs/ft<sup>2</sup>-sec).

XTKE: Product of the temperature in  $^{\circ}\text{K}$  and  $1/EK$ .

YCOMP(I,J): Array to store the concentration profile.

Y(I): Mole fraction of species I.

YI(I): Initial mole fraction of species I.

Z: Distance along the decomposition zone or the char zone (ft).

ZINC: Increment of distance at which the temperature profile is stored (ft).

ZMAX: Maximum allowable thickness of the char zone. (Usually 0.25 inches).

ZZ: Distance of  $Z$  in double precision arithmetic (ft).

INDPTH:

This subroutine calculates the physical properties of the virgin material and the pyrolysis gases.

A...E: These are five empirical constants for the heat capacity of the virgin material.

DELTKK: Increment of temperature ( $^{\circ}\text{K}$ ).

PHMCR:

This subroutine computes the heat absorbed by the decomposition of the phenolic resin and phenolic microballoons.

AREA: This is the area generated by a plot of calories versus temperature ( $^{\circ}\text{K}$ ) by the decomposition of phenolic resin during a differential thermal analysis. (1350 cal/ $^{\circ}\text{K}$ ).

AREAl: This is the area generated by a plot of calories versus temperature ( $^{\circ}\text{K}$ ), by the decomposition of phenolic microballoons during a differential thermal analysis. (1464 calories /  $^{\circ}\text{K}$ ).

A(I)...E(I): These are five empirical constants used to fit a curve through a portion of the plot of calories versus temperature for the phenolic resin.

Al(I)...El(I): These are five empirical constants used to fit a curve through a portion of the plot of calories versus temperature for the phenolic microballoons.

DT: Is the temperature difference in  $^{\circ}\text{K}$  from a base temperature of 350  $^{\circ}\text{C}$  9623 $^{\circ}\text{K}$ ). Below 350 $^{\circ}\text{C}$ , decomposition of the virgin material has not been initiated.

DELT: Is the temperature increment ( $^{\circ}\text{K}$ ) for an increment of the Runge-Kutta step.

H: Is the height (in calories) for the plot of calories versus temperature ( $^{\circ}\text{K}$ ).

K6: Is a code used to bypass the read statements. When K6 is one, the data is read in. When K6 is two, the read statements are bypassed.

NUMBER: Is the number of fits used for the plots of calories versus temperature.

QMICRO: Heat absorbed by the decomposition of the phenolic microballoons (calories/gram).

QPHNLC: Heat absorbed by the decomposition of the phenolic resin (calories/gram).

NYLON:

This subroutine calculates the heat absorbed by the decomposition of nylon.

AREA: This is the area generated by a plot of calories versus temperature ( $^{\circ}\text{K}$ ) for the decomposition of nylon (1122 calories /  $^{\circ}\text{K}$ ) during a differential thermal analysis.

QNYLON: Heat absorbed by the decomposition of nylon (calories/gram).

DENSITY:

This subroutine calculates the density change of phenolic nylon and the mass flux of the pyrolysis gas.

A(J): Frequency factor of reaction J ( $\text{sec}^{-1}$ ).

COMPST: Is an integer variable giving the number of

composite in the ablator. In the case of phenolic nylon, it is three.

DELFLX(I): Is the change in mass flux of composite I due to degradation ( $\text{lbs/ft}^2\text{-sec}$ ).

DRHO: Differential change in density due to degradation. This variable is used as a criteria for stability while the solution is marching through the decomposition zone ( $\text{lbs/ft}^3$ ).

DRHODT(I): Rate of gas generation by the degradation of composite I ( $\text{lbs/ft}^3\text{-sec}$ ).

E(J): Energy of activation of reaction J used to describe the degradation of the composite (Joules/gram-mole).

MASFLX(I): Rate of change of mass flux due to the degradation of composite I ( $\text{lbs/ft}^2\text{-sec}$ ).

MASFRC(I): Mass fraction of each composite in the mixture of virgin material.

NREACT: Number of pseudo-order kinetic reactions used to describe the decomposition of the virgin material composite.

RATER(J): Specific reaction velocity of reaction J ( $\text{lbs/ft}^3\text{-sec}$ ).

RHO: Bulk density of the composite ( $\text{lbs/ft}^3$ ).

RHOC(I): Residual density of composite I ( $\text{lbs/ft}^3$ ).

RHOCC(I): Lowest value of residual density of composite I ( $\text{lbs/ft}^3$ ).

RHOI(I): Initial density of composite I ( $\text{lbs/ft}^3$ ).

RHOII: Initial density of the virgin composite,  
(lbs/ft<sup>3</sup>).

RHOT(I): Density of composite I at temperature T,  
(lbs/ft<sup>3</sup>).

VOLFR(I): Volume fraction of each composite I.

CHARPR:

This subroutine calculates the effective thermal conductivity and the heat capacity of the char.

T: Temperature in °R.

INTRPL:

This program performs Lagrangian interpolation with non-equal step size between points.

F: Dependent variable array.

IMAX: Number of points in array.

SOM: Value of the interpolated dependent variable.

VAR: Value of X for which corresponding value of F is derived by interpolation.

X: Independent variable array.

THERM2:

This subroutine calculates the heat of formation of each chemical species, the heat capacity of the mixture and the heat absorbed by chemical reactions.

CPDT1: Is the sensible enthalpy gain by the constituent elements from a reference temperature of 298.16°K (cal/gram-mole).



CPMX: Heat capacity of the gas mixture (calories/gram-mole  $^{\circ}\text{K}$ ).

ENT1(I): Enthalpy of species I (caloreis/gram-mole).

ENT(I): Heat of formation of species I (cal/gram-mole).

HEAT1: Rate of heat generated, or absorbed, by the chemical reactions (calories/cm<sup>3</sup>-sec).

#### KINET:

This program computes the rate of reaction of each chemical species.

AEF(J): Activation energy of reaction J (calories/gram-mole).

AF(J): Frequency factor of reaction J (sec<sup>-1</sup>

DELZZ: Runge-Kutta step size (cm.).

DLFLUX(I): Differential change in molal flux due to the chemical reaction of species I. This variable is used for the purpose of controlling the step size (gram-mole/cm<sup>2</sup>-sec).

FK(J): Forward reaction rate constant of reaction J.

FLUXMA(I): Mass flux of each chemical species I (gm/cm<sup>2</sup>-sec).

FLUXMO(I): Molal flux of each chemical species I, (gram/moles/cm<sup>2</sup>-sec).

HEAT: Rate of heat generated or absorbed by the chemical reactions (BTU/ft<sup>3</sup>-sec).

K2: Is a counter to keep track of the number of temperature points stored in Table (I,J).

K7: When K7 is one, initialization occurs and sub-routine INOUT is called. When it is 2, this is bypassed.

KOS: Total number of variables stored in the Table (I,J) array.

KSP: Number of gas components in the chemical system.

KSP1: Number of gas and solid species in the chemical system.

NPEX(I,J): Power on the concentration of product I in reaction J.

NREX(I,J): Power on the concentration of reactant I in reaction J.

P: Pressure of the system in atmosphere.

PERCE(J): Mole percent of specie J.

PSC(I,J): Stoichiometric coefficient of the product I in reaction J.

R: Gas constant (82.06 cm<sup>3</sup>-atm/gram-mole °K).

RATE(J): Rate of formation of species I (gram-moles/cm<sup>3</sup>-sec).

RATER(J): Specific reaction velocity of reaction J, (gram-moles/cm<sup>3</sup>-sec).

RK(J): Reverse reaction rate constant of reaction J.

RR: Gas constant (1.98726 calories/gram-mole °K).

SF(J): Power on the temperature of the Arrhenius type kinetic expression.

SPCIE1(J): Species identification name.

T: Temperature (°K).

TABLE(I,J): Is an array where I represents the number

of variables stored and J the number of temperature points. The variables stored are in the following order: T, HEAT, WNEW, AVGFW and KSP1 values of Y1(I).

TESS: Is the absolute maximum value of DLFLUX(I). This variable is used in controlling the step size for stability.

TF: Temperature ( $^{\circ}\text{F}$ ).

TPREV: Is the previous value of the temperature ( $^{\circ}\text{K}$ ).

WNEW: Total mass flux of the gases ( $\text{lbs/ft}^2\text{-sec}$ ).

XMW (I): Molecular weight of species I.

Y1(I): Mole fraction of species I.

#### INPUT1:

This subroutine reads in the kinetic data.

AK(J): Empirical constant for the fit of the equilibrium constant with temperature.

BK(J): Empirical constant for the fit of the equilibrium constant with temperature.

EKMAX(J): Maximum allowable value for the equilibrium constant of reaction J.

EKMIN(J): Minimum allowable value for the equilibrium constant of reaction J.

NCOEF(J): Is the sum of the stoichiometric coefficient of the products minus the reactants.

INPUT FORMAT: A Typical Input For Non-Equilibrium Flow\*

<u>CARD 1:</u>	<u>FORMAT (6I6, F10.1)</u>	<u>COLUMNS</u>
NC = 18		1-6
NNS = 1		7-12
MM = 4		13-18
KODE = 1		19-24
KEY = 3		25-30
INDPT = 0		31-36
TFMAX = 5500		37-46
<u>CARD 2:</u>	<u>FORMAT (F10.3, 10 x, 4F10.3)</u>	
PL = 2160		1-10
TO = 500		21-30
EPS = .30		31-40
ZL = .350000		41-50
HI = .0000001		51-60
<u>CARD 3:</u>	<u>FORMAT (3E15.5, F15.5)</u>	
ALPHA = .5E9		1-15
BETA = .5E5		16-30
SIGMA = .48E-12		31-45
EMIS = .90		46-60

---

\*See Table B-2 for the complete Input data set.

CARD 4:    FORMAT (4E10.3)

## COLUMNS

DTC = 3000

1-10

TCHAR = 1073

11-20

VT = 5.E-4

21-30

CARD 5:   FORMAT (6E10.3,I3)

S1(1) = 1.363250E0

1-10

S2(1) = 1.85605E-3

11-20

S3 (1) = -7.6675E-7

21-30

S4 (1) = .151043E-9

31-40

S5(1) = -1.139E-14

41-50

S6 (1) = -6.49672E2

51-60

```
JCODE(1) = 1
```

61-63

CARD 6: FORMAT (6E10.3)

ALL(1) = -.712442E0

1-10

A22(1) = 7.34065E-3

11-20

A33(1) = -5.526E-6

21-30

A44(1) = 1.51400E-9

31-40

A55(1) = -2.382E-14

41-50

A66 (1) = -6.80533E1

51-60

CARDS 5 and 6 are read sequentially MM times as specified by CARD 1. In this example MM = 4. After CARDS 5 and 6 are read MM times, CARD 7 is read in.

CARD 7: FORMAT (10x, 3E10.3, 2x, 2A3, I4)

```
TLOW(1) = 1000
```

11-20

$$FW(1) = 14.0$$

21-30

YI(1) = 1.0E-71	31-40
SPCIE1(1) = (Blank)	43-45
SPCIE2(1) = CH <sub>2</sub>	46-48
ICODE(1) = 0	49-52

CARD 8:   FORMAT (7E10.3)

AI(1) = 2.229698E0	1-10
BI(1) = 4.71092E-3	11-20
CI(1) = -1.7660E-6	21-30
DI(1) = 3.0649E-10	31-40
EI(1) = -2.017E-14	41-50
FI(1) = 3.383295E4	51-60
GI(1) = 7.707984E0	61-70

CARD 9:

AII(1) = 3.551365E0	1-10
BII(1) = -2.5070E-3	11-20
CII(1) = 1.23550E-5	21-30
DII(1) = 1.175E-08	31-40
EII(1) = 3.8124E-12	41-50
FII(1) = 3.366105E4	51-60
GII(1) = 1.796606E0	61-70

CARD 10:   FORMAT (4E10.3)

AA(1,1) = 1.	1-10
AA(1,2) = 2.0	11-20
AA(1,3) = 0.0	21-30
AA(1,4) = 0.0	31-40

CARD 7, CARD 8, CARD 9 and CARD 10 are read sequentially as a group (NC+NNS) number of times. Only the data for the first species, in this case  $\text{CH}_2$  is presented. The data for other species is given in Table B-2.

<u>CARD 11:</u>	<u>FORMAT (2F15.5)</u>	<u>COLUMNS</u>
EK(1) =	136.5	1-15
SIG(1) =	3.822	16-30

CARD 11 is read NC number of times as specified in CARD 1.

<u>CARD 12:</u>	<u>FORMAT (I6)</u>	
NDATA =	34	1-16

<u>CARD 13:</u>	<u>FORMAT (2F15.5)</u>	
XTKE(1) =	0.30	1-15
ZOMGA(1) =	2.785	16-30

CARD 13 is repeated NDATA number of times as specified by CARD 12.

CARDS 1 through 13 are read in the MAIN program. These cards define the physical condition of the system.

In addition they provide the thermodynamic data and physical constants for the pyrolysis species. CARDS 14 through 19, below, provide the thermophysical information for the virgin material and also for the kinetic data for the degradation of the polymer.

<u>CARD 14:</u>	<u>FORMAT (5E12.6)</u>	<u>COLUMNS</u>
A =	0.37000070E0	1-12
B =	0.7367133E-4	13-24
C =	0.1532518E-5	25-36
D =	-.1962704E-4	37-48
E =	.8857809E-12	49-60

CARD 14 is read in subroutine INDPTH.

<u>CARD 15:</u>	<u>FORMAT (5E12.8)</u>	
A(1) =	0.10561790E0	1-12
B(1) =	-1.836062E-2	13-24
C(1) =	1.7580490E-3	25-36
D(1) =	-1.678598E-5	37-48
E(1) =	4.7310570E-8	49-60

<u>CARD 16:</u>	<u>FORMAT (5E12.8)</u>	
A1(1) =	-.35642660E-1	1-12
B1(1) =	4.5790730E-2	13-24
C1(1) =	1.2298170E-4	25-36
D1(1) =	-.8277667E-7	37-48
E1(1) =	-.2279748E-7	49-60

CARD 15 and CARD 16 are read sequentially four times in subroutine PHMCR. For a thorough explanation of the sources of data for the phenolic resin see Appendix C.

<u>CARD 17:</u>	<u>FORMAT (2I6)</u>	
COMPST		1-6
NREACT		7-12



CARD 18:      FORMAT (4x, I6, 3E10.8)    COLUMNS

I =	5-10
A(J) =	11-20
E(J) =	21-30
XN(I,J) =	31-40

CARD 18 is read NREACT number of times.

CARD 19:      FORMAT (3I0.3)

RHOI(1) =	1-10
RHOC(1) =	11-20
MASFRC(1) =	21-30

CARD 19 is read COMPST number of times. CARDS 17, 18 and 19 are read in subroutine DENSITY.

CARD 20:      FORMAT (I2)

NEQ =	1-2
-------	-----

CARD 21:      FORMAT (19A4)

EQN = Alphameric Reaction Expression    1-76

CARD 22:      FORMAT (6(I2, F3.0))

I =	1-2
RSC(1,I)	3-5
I =	6-7
RSC(1,I)	8-10
I =	11-12
RSC(1,I)	13-15
I =	16-17

	<u>COLUMNS</u>
PSC(1,I)	13-20
I =	21-22
PSC(1,I)	23-25
I =	26-27
PSC(1,I)	28-30

CARD 23:

I =	1-2
NREX(1,I)	3-5
I =	6-7
NREX(1,I)	8-10
I =	11-12
NREX(1,I)	13-15
I =	16-17
NPEX(1,I)	18-20
I =	21-22
NPEX(1,I)	23-25
I =	26-27
NPEX(1,I)	28-30

CARD 24:   FORMAT (E8.0, 2x, 2F10.1)

AF(1) =	1-8
SF(1) =	11-20
AEF(1) =	21-30

<u>CARD 25:</u> <u>FORMAT</u> (4E15.7, I5)	<u>COLUMNS</u>
AK(1)	1-15
BK(1)	16-30
EKMAX(1)	31-45
NCOEF(1)	46-50

CARDS 21,22,23,24 and 25 are read sequentially NEQ number of times.

In CARD 22, J = 1 through 18 corresponds respectively to the following species: CH<sub>2</sub>, CH<sub>3</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H, H<sub>2</sub>, H, N<sub>2</sub>, C<sub>6</sub>H<sub>6</sub>O, C<sub>6</sub>H<sub>6</sub>, NH<sub>3</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, OH, O, C.

TABLE B-5. Listing of Typical Input Data for Non-Equilibrium Analysis

18	1	4	1	3	1	0			DATA	1
2160.				500.		.8	0.3500000	.00000001	5821.	DATA 2
.50000E9			.50000E5		.481E-12	0.90				DATA 3
1.363252E01	1.85605E-3	-7.6675E-7	1.51043E-9	-1.139E-14	-6.49672E2	1				DATA 4
-.712442E07	7.34065E-3	-5.5262E-6	1.51400E-9	-2.382E-14	-6.80533E1					DATA 5
3.043690E06	6.11871E-4	-7.3994E-9	-2.033E-11	2.4594E-15	-8.54910E2	0				DATA 6
1.00000E0	4.00000E00	0.00000E00	0.00000E00							DATA 7
	1000.E0	30.070E0		.0034	C2H6	0				DATA 8
.1430799E1	1.188898E-1	-.70440E-5	1.18720E-8	-.7445E-13	-.114311E5	1.401321E2				DATA 9
.2882039E1	1.103219E-1	1.119142E-4	-.14832E-7	4.4749E-11	-.116209E5	7.597900E1				DATA 10
2.00000E0	6.00000E0	0.00000E0	0.00000E0							DATA 11
	1000.E0	28.054E0		.0218	C2H4	0				DATA 12
3.5023E00	1.159E-02	-4.4745E-6	7.945E-10	-5.323E-14	4.5439E03	2.4667E00				DATA 13
1.120244E0	1.3906E-2	2.6568E-6	-1.1560E-85	2.387E-125	3.32889E3	1.58378E1				DATA 14
2.00000E0	4.00000E0	0.00000E0	0.00000E0							DATA 15
	1000.E0	26.038E0		.0233	C2H2	0				DATA 16
4.4966E00	5.2698E-3	-1.840E-063	1.054E-10	-2.000E-142	5.637E004	-3.14481E0				DATA 17
7.90333E-1	2.3466E-2	-3.5542E-5	2.7951E-8	-8.448E-12	2.6255E04	1.4005E01				DATA 18
2.00000E0	2.00000E0	0.00000E0	0.00000E0							DATA 19
	1000.E0	25.030E0	1.00E-71		C2H	0				DATA 20
.3513479E1	1.358906E-2	-.13231E-5	2.30520E-9	-.1530E-13	5.788759E5	5.4523285E1				DATA 21
.3006269E1	1.553788E-2	-.35112E-5	1.24860E-8	-.1896E-12	5.796960E5	6.920349E1				DATA 22
2.00000E0	1.00000E0	0.00000E0	0.00000E0							DATA 23
	1000.E0	2.016E0		.2372	H2	0				DATA 24
3.04369E00	6.1187E-4	-7.399E-9	-2.03E-11	2.459E-15	-8.5491E02	-1.648E00				DATA 25
2.846085E04	1.932E-03	-9.6119E-69	5.123E-09	-3.309E-12	-9.67254E2	-1.4118E0				DATA 26
0.000000E0	2.00000E0	0.00000E0	0.00000E0							DATA 27
	1000.E0	1.008E0	1.000E-71		H	0				DATA 28
2.500000E0	0.00000E0	0.00000E0	0.00000E0	0.00000E02	5.47050E4	-4.6001E-1				DATA 29
2.500000E0	0.00000E0	0.00000E0	0.00000E0	0.00000E02	5.47050E4	-4.6001E-1				DATA 30
0.000000E0	1.00000E0	0.00000E0	0.00000E0							DATA 31
	1000.E0	28.016E0		.0277	N2	0				DATA 32
2.854576E0	1.5976E-3	-6.2566E-71	1.1316E-10	-7.69E-15	-8.90174E2	6.39029E0				DATA 33
										DATA 34

3.691615E0-1.3333E-32.65031E-6-9.769E-10-9.977E-14-1.06283E3 2.28750E0	DATA	35
0.000000E0 0.000000E0 2.000000E0 0.000000E0	DATA	36
1500.E0 94.114E0 .0385 C6H6O 0	DATA	37
-3.93169E06.93818E-2-5.2106E-51.24967E-82.0915E-12-1.33038E44.187817E1	DATA	38
-3.93169E06.93818E-2-5.2106E-51.24967E-82.0915E-12-1.33038E44.187817E1	DATA	39
6.000000E0 6.000000E0 0.000000E0 1.000000E0	DATA	40
1500.E0 78.114E0 .0052 C6H6 0	DATA	41
.3511186E03.75399E-2-7.9473E-6-7.5092E-93.0385E-128.264418E31.986606E1	DATA	42
4.619872E02.88096E-2-1.1245E-51.95764E-9-1.257E-137.391621E4-1.78947E0	DATA	43
6.000000E0 6.000000E0 0.000000E0 0.000000E0	DATA	44
1000.E0 17.032E0 1.00E-71 NH3 0	DATA	45
2.149399E06.49285E-3-2.2695E-63.7394E-10-2.361E-14-6.40196E3 9.23891E0	DATA	46
3.77162E00-4.8621E-49.8742E-06-9.5679E-93.1313E-12-6.72810E3 1.4654E00	DATA	47
0.000000E00 3.000000E0 1.000000E0 0.000000E0	DATA	48
1000.E0 28.011E0 .0233 CO 0	DATA	49
2.9512E00 1.5526E-3-6.1911E-7 1.135E-10-7.788E-15-1.4232E04 6.5314E00	DATA	50
3.787133E0-2.171E-035.07573E-6-3.4738E-97.7217E-13-1.43635E4 2.63355E0	DATA	51
1.000000E0 0.000000E0 0.000000E0 1.000000E0	DATA	52
1000.E0 44.011E0 .0164 CO2 0	DATA	53
4.4129E003.1923E-03 -1.298E-6 2.415E-10-1.674E-14-4.8944E04-7.2876E-1	DATA	54
2.170100E0 1.0378E-2-1.0734E-56.34592E-9-1.628E-12-4.83526E4 1.06644E1	DATA	55
1.000000E0 0.000000E0 0.000000E0 2.000000E0	DATA	56
1000.E0 18.016E0 .0492 H2O 0	DATA	57
2.67075E0 3.0317E-3 -8.535E-7 1.179E-10-6.197E-15-2.9889E04 6.88383E0	DATA	58
4.15650E00-1.7244E-35.6982E-06-4.5930E-91.4234E-12-3.02888E4-6.8616E-1	DATA	59
0.000000E0 2.000000E0 0.000000E0 1.000000E0	DATA	60
1000.E0 17.008E0 1.000E-71 OH 0	DATA	61
2.889554E09.98350E-4-2.1880E-71.9803E-11-3.845E-163.881179E35.559701E0	DATA	62
3.823470E0-1.1187E-31.24668E-6-2.103E-10-5.254E-143.585278E35.8253E-01	DATA	63
0.000000E0 1.000000E0 0.000000E0 1.000000E0	DATA	64
1000.E0 16.000000 1.00E-71 O O	DATA	65
2.537256E0-1.8422E-5-8.8018E-95.9643E-12-5.574E-162.92300E044.946794E0	DATA	66
3.021889E0-2.1737E-33.75422E-6-2.9947E-99.0777E-132.913719E42.646007E0	DATA	67
0.0000E00 0.00000E0 0.0000E00 1.0000E00	DATA	68

1000.E0	12.011E0	.515	C	1	DATA	69		
1.36325E00	1.85605E-3	-7.6675E-7	1.5104E-10	-1.139E-14	-6.4967E02	-7.9890E00	DATA	70
-7.1244E-17	3.4065E-3	-5.5262E-6	1.514E-09	-2.382E-14	-6.80533E1	2.79326E0	DATA	71
1.0000E00	0.0000E0	0.0000E00	0.0000E00				DATA	72
136.5		3.822	CH2				DATA	73
136.5		3.822	CH3				DATA	74
136.5		3.822	CH4				DATA	75
230.0		4.418	C2H6				DATA	76
205.0		4.232	C2H4				DATA	77
185.0		4.221	C2H2				DATA	78
185.0		4.221	C2H				DATA	79
33.3		2.986	H2				DATA	80
33.3		2.986	H				DATA	81
91.5		3.681	N2				DATA	82
440.0		5.270	C6H6				DATA	83
400.0		5.000	PHOH				DATA	84
312.0		3.432	NH3				DATA	85
110.0		3.590	CO				DATA	86
190.0		3.996	CO2				DATA	87
356.0		2.649	H2O				DATA	88
113.0		3.433	OH				DATA	89
113.0		3.433	O				DATA	90
34							DATA	91
0.30		2.785					DATA	92
0.35		2.628					DATA	93
2.846085E04	1.9321E-3	-9.6119E-69	5.1227E-9	-3.309E-12	-9.67253E2		DATA	94
3.691615E0	-1.3333E-32	6.5031E-6	-.97688E-9	-9.977E-14	-1.06283E3		DATA	95
3.597613E07	8.1456E-4	-2.2387E-74	2.490E-11	-3.346E-15	-1.19279E3	0	DATA	96
2.854576E01	5.9763E-3	-6.2566E-7	1.13158E-9	-7.690E-15	-8.90174E2	0	DATA	97
3.718995E0	-2.5167E-38	5.8374E-6	-8.2999E-92	7.082E-12	-1.10577E3		DATA	98
1000.E0	14.00E0	1.000E-71	CH2	0			DATA	99
2.229698E04	7.1092E-3	-1.7660E-63	0.649E-10	-2.017E-143	3.83295E47	7.07984E0	DATA	100
3.551365E0	-2.5070E-31	2.3550E-5	-1.175E-083	8.124E-123	3.66105E41	7.96606E0	DATA	101
1.000000E0	2.00000E0	0.00000E0	0.00000E0				DATA	102

1000.E0	15.035E0	1.000E-71	CH3	0	DATA 103
2.802766E06	2.5045E-3	2.2892E-63	8.993E-10	2.528E-141	5.78749E45.684117E0
3.399505E04	2.6783E-32	0.03327E-7	1.1548E-94	0.1288E-131	5.64979E42.703747E0
1.000000E0	3.00000E0	0.00000E0	0.00000E0	0.00000E0	DATA 106
1000.E0	16.043E0	.039	CH4	0	DATA 107
1.18000E0	1.0950E-2	4.0620E-6	7.137E-10	4.749E-14	9.8556E03 1.2506E01
4.249768E0	6.9127E-3	3.1602E-5	2.9715E-89	5.103E-12	1.01866E4-9.1755E-1
0.40	2.492				DATA 110
0.45	2.368				DATA 111
0.50	2.257				DATA 112
0.55	2.156				DATA 113
0.60	2.065				DATA 114
0.65	1.982				DATA 115
0.70	1.908				DATA 116
0.75	1.841				DATA 117
0.80	1.780				DATA 118
0.85	1.725				DATA 119
0.90	1.675				DATA 120
0.95	1.629				DATA 121
1.00	1.587				DATA 122
1.10	1.514				DATA 123
1.20	1.452				DATA 124
1.30	1.399				DATA 125
1.50	1.314				DATA 126
1.70	1.248				DATA 127
1.90	1.197				DATA 128
2.2	1.138				DATA 129
2.6	1.081				DATA 130
3.2	1.022				DATA 131
4.0	0.9700				DATA 132
5.0	0.9269				DATA 133
7.0	0.8727				DATA 134
10.0	0.8242				DATA 135
20.0	0.7432				DATA 136

40.0	0.6718				DATA 137
70.0	0.6194				DATA 138
100.0	0.5882				DATA 139
200.0	0.5320				DATA 140
400.0	0.4811				DATA 141
0.3700070E0 0.7367133E-4 .1532518E-5-.1962704E-8.8857809E-12					DATA 142
3	7				DATA 143
1	8.3000E14	232.000E0	1.00000E0		DATA 144
2	5.10000E8	114.000E0	3.00000E0		DATA 145
2	2.50000E5	100.000E0	1.30000E0		DATA 146
2	2.00000E7	140.000E0	3.10000E0		DATA 147
3	2.00000E5	70.000E0	2.00000E0		DATA 148
3	9.70000E6	122.000E0	2.00000E0		DATA 149
3	1.3000E10	172.000E0	3.00000E0		DATA 150
68.6000E0 5.14500E0 0.4000E0					DATA 151
80.0000E0 43.2800E0 0.2500E0					DATA 152
17.8000E0 9.64760E0 0.3500E0					DATA 153
15	19				DATA 154
CH4=CH2+H2(1670-2090 K)KOZLOV, RUSSIAN J. PHYS. CHEM. VOL 37, SEP. 1963, 1-1-4					DATA 155
3	1. 30 0. 30 0.	1 1. 8 1. 30 0.			DATA 156
3	1 30 0 30 0	1 1 8 1 30 0			DATA 157
4.5E+13	0.	91.			DATA 158
0.1664396E+2	-0.4365610E+5	4.0E0	1.E-6	1	DATA 159
CH4=CH3+H(1590-1750 K)					DATA 160
3	1. 30 0. 30 0.	2 1. 9 1. 30 0.			DATA 161
3	1 30 0 30 0	2 1 9 1 30 0			DATA 162
1.0E+15	0.	103.			DATA 163
0.1725283E+2	-0.5315890E+5	10.0E0	1.E-6	1	DATA 164
2CH3=C2H6					DATA 165
2	2. 30 0. 30 0.	4 1. 30 0. 30 0.			DATA 166
2	2 30 0 30 0	4 1 30 0 30 0			DATA 167
1.5E+10	0.	28.2			DATA 168
-0.2030537E+2	0.4381153E+5	1.E+10	5.2E-4	-1	DATA 169
C2H6=C2H4+H2(1600-3700 K), G.V. GULYAEV, 1-10					DATA 170



4 1. 30 0. 30 0. 5 1. 8 1. 30 0.				DATA 171
4 1 30 0 30 0 5 1 8 1 30 0				DATA 172
9.0E+13 0. 69.0				DATA 173
0.1604147E+2 -0.1715366E+5	1.E+4	1.E-1	1	DATA 174
C2H4=C2H2+H2(1300-2000 K),RUSSIAN J.PHYS.CHEM.,P1128-1130,SEP1963 *				DATA 175
5 1. 30 0. 30 0. 6 1. 8 1. 30 0.				DATA 176
5 1 30 0 30 0 6 1 8 1 30 0				DATA 177
1.1E+13 0.0 72.0				DATA 178
0.1538761E+2 -0.2100359E+5	2.1E4	1.E-8	1	DATA 179
C2H2=2C+H2(2000 K)GULYAEV,INST.OF PET SYNTHESIS,ACAD.OF SCI.,USSR,I-10				DATA 180
6 1. 30 0. 30 0. 19 2. 8 1. 30 0.				DATA 181
6 1 30 0 30 0 19 0 8 1 30 0				DATA 182
1.7E+06 0. 30.				DATA 183
-0.5979611E+1 0.2595788E+5	2.E+8	4.17E0	0	DATA 184
C2H2=C2H+H (INVERTED ORDER)				DATA 185
6 1. 30 0. 30 0. 7 1. 9 1. 30 0.				DATA 186
6 1 30 0 30 0 7 1 9 1 30 0				DATA 187
4.5E+11 0. 35.5				DATA 188
0.1603705E+2 -0.5805091E+5	1.E12	1.0E-2	1	DATA 189
C+H2O=CO+H2				DATA 190
19 1. 16 1. 30 0. 14 1. 8 1. 30 0.				DATA 191
19 0 16 1 30 0 14 1 8 1 30 0				DATA 192
2.3E+11 -0.50 71.9				DATA 193
0.1717660E+2 -0.1626795E+5	8.35E4	1.37E-7	1	DATA 194
C+CO2=2CO				DATA 195
19 1. 15 1. 30 0. 14 2. 30 0. 30 0.				DATA 196
19 0 15 1 30 0 14 2 30 0 30 0				DATA 197
1.5E+10 0. 85.				DATA 198
0.2068290E+2 -0.2015984E+5	1.57E5	1.E-06	1	DATA 199
H2+M=2H+M LWP-181 I-1, 2-1				DATA 200
8 1. 20 1. 30 0. 9 2. 20 1. 30 0.				DATA 201
8 1 20 1 30 0 9 2 20 1 30 0				DATA 202
3.6E+18 0.82 103.2				DATA 203
0.1465827E+2 -0.5507806E+5	.3450	1.E-11	1	DATA 204

H2O+M=OH+H LWP(300-3250 K)				DATA 205
16 1. 20 1. 30 0. 17 1. 9 1. 30 0.				DATA 206
16 1 20 1 30 0 17 1 9 1 30 0				DATA 207
1.7E+22 1.31 118.0				DATA 208
0.1575620E+2 -0.6166211E+5	0.35E0	1.E-14	1	DATA 209
H+C02=C0+OH(1273-2273 K)				DATA 210
9 1. 15 1. 30 0. 14 1. 17 1. 30 0.				DATA 211
9 1 15 1 30 0 14 1 17 1 30 0				DATA 212
3.0E+12 0. 33.				DATA 213
0.4460376E+1 -0.1056866E+5	3.85E0	1.E-9	0	DATA 214
C02=C0+O(HARPER-BOEING) LWP 181 II-2				DATA 215
15 1. 30 0. 30 0. 14 1. 18 1. 30 0.				DATA 216
15 1 30 0 30 0 14 1 18 1 30 0				DATA 217
2.3E+11 -0.5 71.9				DATA 218
0.1787079E+2 -0.6348669E+5	0.766E0	5.076E-14	1	DATA 219
C6H6O+H2=H2O+C6H6 APRIL ,PH.D. THESIS. MAY 1969				DATA 220
11 1. 8 1. 30 0. 16 1. 12 1. 30 0.				DATA 221
11 1 8 1 30 0 16 1 12 1 30 0				DATA 222
2.0E+13 0. 45.				DATA 223
-0.5793374E-1 0.8101410E+4	1.00E+7	1.000E-5	0	DATA 224
C6H6=3C2H2 APRIL ,PH.D. THESIS. MAY 1969				DATA 225
12 1. 30 0. 30 0. 6 3. 30 0. 30 0.				DATA 226
12 1 30 0 30 0 6 3 30 0 30 0				DATA 227
1.4E+09 0. 52.				DATA 228
0.3830254E+2 -0.6562874E+5	1.0E+10	1.0E-08	2	DATA 229

**TABLE B-6. Typical Output for Non-Equilibrium**

**INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)**

**THEORETICAL**

CHAR BACK TEMPERATURE (OF)= 1471.7	NUMBER OF GAS COMPONENTS= 18
THICKNESS OF CHAR(INCHES)=0.020672	THICKNESS OF DECOMPOSITION ZONE=0.006869
TOTAL MASS FLUX(LBS/FT2-SEC)=.349420	GAS MASS FLUX AT THE SURFACE= .168964
FRONT SURFACE TEMPERATURE(OF)=5500.0	SURFACE RECESSION VELOCITY(FT/SEC)=0.01000
RATE OF HEAT ABSORBED IN THE CHAR ZONE(BTU/FT2-SEC)=1711.8933	
RATE OF HEAT ABSORBED IN THE DECOMPOSITION ZONE(BTU/FT2-SEC)= 244.2668	
PERCENT OF TOTAL HEAT ABSORBED IN THE CHAR ZONE= 0.8751294E 02	
PERCENT OF TOTAL HEAT ABSORBED IN DECOMP-ZONE= 0.1248705E 02	
PERCENT OF HEAT ABSORBED BY THE GAS IN THE CHAR ZONE= 0.4130847E 02	
PERCENT OF HEAT ABSORBED BY THE SOLIDS IN THE CHAR ZONE= 0.2505246E 02	
PERCENT OF HEAT ABSORBED BY REACTION IN THE CHAR ZONE= 0.3363907E 02	

# INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

TEMPERATURE DROP (OF) = 4028.4

PRESSURE DROP (LB/FT2) = 9.1

SURFACE HEAT FLUX (BTU/FT2-SEC) = 1956.16

RADIANT HEAT FLUX (BTU/FT2-SEC)=, 546.15

AERODYNAMIC HEAT FLUX(BTU/FT2-SEC)= 2502.31

CHAR DEPTH (FT)	0.0006	0.0006	0.0007	0.0007	0.0007
TEMPERATURE (OF)	1471.7	1556.4	1648.1	1746.2	1848.7
PRESSURE (LB/FT2)	2169.1	2168.9	2168.6	2168.4	2168.2
MASS FLUX(LB/FT2-SEC)	0.1285	0.1606	0.1606	0.1606	0.1606

## GAS COMPONENT

## COMPOSITION (MOLE/MOLE GAS)

1	CH2	0.1000E-70	0.3100E-10	0.2112E-09	0.2614E-08	0.1767E-07
2	CH3	0.1000E-70	0.3152E-11	0.2733E-10	0.4766E-09	0.4591E-08
3	CH4	0.8250E-01	0.8141E-01	0.8098E-01	0.8100E-01	0.8100E-01
4	C2H6	0.7390E-02	0.7292E-02	0.7254E-02	0.7253E-02	0.7245E-02
5	C2H4	0.4739E-01	0.4676E-01	0.4651E-01	0.4652E-01	0.4654E-01
6	C2H2	0.5103E-01	0.3705E-01	0.3163E-01	0.3184E-01	0.3194E-01
7	C2H	0.1000E-70	0.1330E-01	0.1846E-01	0.1826E-01	0.1816E-01
8	H2	0.4400E 00	0.4342E 00	0.4319E 00	0.4320E 00	0.4320E 00
9	H	0.1000E-70	0.1330E-01	0.1846E-01	0.1826E-01	0.1816E-01
10	N2	0.4751E-01	0.4688E-01	0.4663E-01	0.4664E-01	0.4665E-01
11	C6H60	0.8393E-01	0.8281E-01	0.8238E-01	0.8240E-01	0.8240E-01
12	C6H6	0.1128E-01	0.1113E-01	0.1107E-01	0.1108E-01	0.1108E-01
13	NH3	0.1000E-70	0.9867E-71	0.9815E-71	0.9817E-71	0.9818E-71
14	CO	0.5677E-01	0.5601E-01	0.5572E-01	0.5573E-01	0.5574E-01
15	CO2	0.3574E-01	0.3526E-01	0.3508E-01	0.3508E-01	0.3509E-01
16	H2O	0.1364E 00	0.1346E 00	0.1339E 00	0.1339E 00	0.1340E 00
17	OH	0.1000E-70	0.1085E-07	0.5764E-07	0.2389E-06	0.6032E-06
18	O	0.1000E-70	0.1109E-09	0.1103E-09	0.1104E-09	0.1104E-09
19	C	0.1110E 01	0.1095E 01	0.1089E 01	0.1089E 01	0.1090E 01

# INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0008	0.0008	0.0009	0.0009	0.0010
TEMPERATURE (OF)	1953.8	2063.0	2172.5	2283.7	2396.5
PRESSURE (LB/FT2)	2168.0	2167.7	2167.5	2167.3	2167.1
MASS FLUX(LB/FT2-SEC)	0.1606	0.1606	0.1607	0.1607	0.1608

## GAS COMPONENT

## COMPOSITION (MOLE/MGLE GAS)

1	CH2	0.2192E-06	0.1000E-69	0.1734E-05	0.7617E-05	0.1632E-04
2	CH3	0.7686E-07	0.1000E-69	0.8569E-06	0.4981E-05	0.1114E-04
3	CH4	0.8099E-01	0.8101E-01	0.8093E-01	0.8079E-01	0.8060E-01
4	C2H6	0.7169E-02	0.7163E-02	0.6793E-02	0.6194E-02	0.5357E-02
5	C2H4	0.4659E-01	0.4662E-01	0.4682E-01	0.4713E-01	0.4757E-01
6	C2H2	0.3195E-01	0.3192E-01	0.3201E-01	0.3216E-01	0.3238E-01
7	C2H	0.1815E-01	0.1816E-01	0.1814E-01	0.1811E-01	0.1807E-01
8	H2	0.4321E 00	0.4321E 00	0.4325E 00	0.4332E 00	0.4341E 00
9	H	0.1815E-01	0.1812E-01	0.1815E-01	0.1822E-01	0.1832E-01
10	N2	0.4664E-01	0.4665E-01	0.4660E-01	0.4653E-01	0.4643E-01
11	C6H6O	0.8239E-01	0.8239E-01	0.8231E-01	0.8218E-01	0.8199E-01
12	C6H6	0.1108E-01	0.1109E-01	0.1108E-01	0.1107E-01	0.1105E-01
13	NH3	0.9816E-71	0.9818E-71	0.9809E-71	0.9794E-71	0.9772E-71
14	CO	0.5579E-01	0.5571E-01	0.5603E-01	0.5659E-01	0.5741E-01
15	CO2	0.3508E-01	0.3513E-01	0.3504E-01	0.3486E-01	0.3459E-01
16	H2O	0.1339E 00	0.1340E 00	0.1335E 00	0.1327E 00	0.1315E 00
17	OH	0.2018E-05	0.1000E-69	0.1804E-04	0.1105E-03	0.2490E-03
18	O	0.1103E-09	0.1000E-69	0.1449E-04	0.1392E-03	0.3274E-03
19	C	0.1089E 01	0.1090E 01	0.1088E 01	0.1086E 01	0.1083E 01

# INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0010	0.0011	0.0011	0.0011	0.0012
TEMPERATURE (OF)	2513.6	2628.5	2744.1	2860.4	2976.0
PRESSURE (LB/FT2)	2166.9	2166.6	2166.4	2166.2	2166.0
MASS FLUX(LB/FT2-SEC)	0.1607	0.1609	0.1612	0.1616	0.1622

GAS COMPONENT		COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.9922E-05	0.3263E-04	0.6520E-04	0.1081E-03	0.1730E-03
2	CH3	0.3257E-04	0.3727E-04	0.3926E-04	0.3988E-04	0.7375E-04
3	CH4	0.8058E-01	0.8016E-01	0.7958E-01	0.7885E-01	0.7782E-01
4	C2H6	0.3694E-02	0.2602E-02	0.1467E-02	0.3201E-03	0.9261E-04
5	C2H4	0.4981E-01	0.4975E-01	0.4918E-01	0.4805E-01	0.4501E-01
6	C2H2	0.3180E-01	0.3255E-01	0.3369E-01	0.3524E-01	0.3756E-01
7	C2H	0.1807E-01	0.1798E-01	0.1786E-01	0.1771E-01	0.1750E-01
8	H2	0.4340E 00	0.4361E 00	0.4388E 00	0.4423E 00	0.4463E 00
9	H	0.1771E-01	0.1823E-01	0.1906E-01	0.2025E-01	0.2257E-01
10	N2	0.4643E-01	0.4620E-01	0.4589E-01	0.4549E-01	0.4495E-01
11	C6H6O	0.8200E-01	0.8158E-01	0.8101E-01	0.8028E-01	0.7931E-01
12	C6H6	0.1105E-01	0.1100E-01	0.1094E-01	0.1085E-01	0.1074E-01
13	NH3	0.9773E-71	0.9725E-71	0.9659E-71	0.9575E-71	0.9462E-71
14	CO	0.5692E-01	0.5895E-01	0.6185E-01	0.6564E-01	0.7105E-01
15	CO2	0.3393E-01	0.3362E-01	0.3332E-01	0.3304E-01	0.3265E-01
16	H2O	0.1333E 00	0.1299E 00	0.1249E 00	0.1181E 00	0.1080E 00
17	OH	0.1000E-69	0.2156E-03	0.1173E-02	0.2516E-02	0.5017E-02
18	O	0.9881E-03	0.1132E-02	0.1193E-02	0.1172E-02	0.1159E-02
19	C	0.1084E 01	0.1077E 01	0.1066E 01	0.1053E 01	0.1034E 01

# INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0012	0.0013	0.0013	0.0014	0.0014
TEMPERATURE (OF)	3092.2	3210.0	3329.7	3449.6	3567.1
PRESSURE (LB/FT2)	2165.7	2165.5	2165.3	2165.0	2164.8
MASS FLUX(LB/FT2-SEC)	0.1639	0.1660	0.1673	0.1682	0.1685

GAS COMPONENT		COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.3888E-03	0.7688E-03	0.1362E-02	0.2495E-02	0.4413E-02
2	CH3	0.1436E-03	0.2467E-03	0.4062E-03	0.7837E-03	0.1526E-02
3	CH4	0.7485E-01	0.7101E-01	0.6788E-01	0.6487E-01	0.6145E-01
4	C2H6	0.1252E-04	0.5737E-05	0.2738E-05	0.8772E-06	0.1700E-06
5	C2H4	0.3584E-01	0.2418E-01	0.1454E-01	0.5890E-02	0.1482E-02
6	C2H2	0.4404E-01	0.5225E-01	0.5949E-01	0.6673E-01	0.7059E-01
7	C2H	0.1690E-01	0.1614E-01	0.1561E-01	0.1528E-01	0.1511E-01
8	H2	0.4558E 00	0.4656E 00	0.4724E 00	0.4795E 00	0.4842E 00
9	H	0.3114E-01	0.4408E-01	0.5338E-01	0.5617E-01	0.5636E-01
10	N2	0.4341E-01	0.4148E-01	0.4011E-01	0.3925E-01	0.3881E-01
11	C6H6O	0.7651E-01	0.7299E-01	0.7047E-01	0.6880E-01	0.6782E-01
12	C6H6	0.1040E-01	0.9979E-02	0.9688E-02	0.9529E-02	0.9475E-02
13	NH3	0.9137E-71	0.8730E-71	0.8442E-71	0.8260E-71	0.8168E-71
14	CO	0.8547E-01	0.1013E 00	0.1106E 00	0.1161E 00	0.1186E 00
15	CO2	0.3153E-01	0.3012E-01	0.2913E-01	0.2850E-01	0.2818E-01
16	H2O	0.7827E-01	0.4099E-01	0.1654E-01	0.4952E-02	0.1275E-02
17	OH	0.1412E-01	0.2770E-01	0.3737E-01	0.4012E-01	0.3974E-01
18	O	0.1119E-02	0.1069E-02	0.1034E-02	0.1012E-02	0.1000E-02
19	C	0.9818E 00	0.9185E 00	0.8758E 00	0.8494E 00	0.8366E 00

# INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0015	0.0015	0.0015	0.0016	0.0016
TEMPERATURE (OF)	3681.8	3793.8	3903.2	4010.5	4115.6
PRESSURE (LB/FT2)	2164.6	2164.3	2164.1	2163.9	2163.6
MASS FLUX(LB/FT2-SEC)	0.1686	0.1686	0.1686	0.1686	0.1685

## GAS COMPONENT

## COMPOSITION (MOLE/MOLE GAS)

1	CH2	0.7336E-02	0.1115E-01	0.1608E-01	0.2132E-01	0.2673E-01
2	CH3	0.2718E-02	0.4308E-02	0.6392E-02	0.8602E-02	0.1089E-01
3	CH4	0.5686E-01	0.5102E-01	0.4345E-01	0.3540E-01	0.2708E-01
4	C2H6	0.2384E-07	0.4605E-08	0.3111E-08	0.1715E-08	0.1804E-08
5	C2H4	0.2476E-03	0.6069E-04	0.4416E-04	0.3552E-04	0.2901E-04
6	C2H2	0.7169E-01	0.7192E-01	0.7207E-01	0.7237E-01	0.7296E-01
7	C2H	0.1500E-01	0.1490E-01	0.1478E-01	0.1464E-01	0.1450E-01
8	H2	0.4862E 00	0.4875E 00	0.4888E 00	0.4902E 00	0.4914E 00
9	H	0.5716E-01	0.5839E-01	0.6003E-01	0.6176E-01	0.6353E-01
10	N2	0.3853E-01	0.3828E-01	0.3796E-01	0.3762E-01	0.3726E-01
11	C6H6D	0.6709E-01	0.6634E-01	0.6542E-01	0.6441E-01	0.6325E-01
12	C6H6	0.9459E-02	0.9437E-02	0.9387E-02	0.9308E-02	0.9190E-02
13	NH3	0.8110E-71	0.8057E-71	0.7990E-71	0.7919E-71	0.7842E-71
14	CO	0.1190E 00	0.1187E 00	0.1181E 00	0.1175E 00	0.1170E 00
15	CO2	0.2797E-01	0.2778E-01	0.2754E-01	0.2728E-01	0.2699E-01
16	H2O	0.2597E-03	0.1016E-03	0.7977E-04	0.6569E-04	0.5428E-04
17	OH	0.3946E-01	0.3920E-01	0.3888E-01	0.3853E-01	0.3816E-01
18	O	0.9932E-03	0.9866E-03	0.9784E-03	0.9697E-03	0.9603E-03
19	C	0.8299E 00	0.8245E 00	0.8179E 00	0.8108E 00	0.8031E 00



# INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0017	0.0017	0.0018	0.0018	0.0019
TEMPERATURE (OF)	4218.6	4319.4	4418.2	4514.8	4609.5
PRESSURE (LB/FT2)	2163.4	2163.2	2162.9	2162.7	2162.5
MASS FLUX(LB/FT2-SEC)	0.1685	0.1685	0.1685	0.1685	0.1684

GAS COMPONENT		COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.3083E-01	0.3420E-01	0.3648E-01	0.3788E-01	0.3868E-01
2	CH3	0.1268E-01	0.1430E-01	0.1562E-01	0.1672E-01	0.1767E-01
3	CH4	0.2068E-01	0.1519E-01	0.1119E-01	0.8278E-02	0.6150E-02
4	C2H6	0.1303E-09	0.3227E-08	0.3910E-08	0.3615E-08	0.5711E-08
5	C2H4	0.2462E-04	0.2100E-04	0.1825E-04	0.1608E-04	0.1428E-04
6	C2H2	0.7381E-01	0.7513E-01	0.7683E-01	0.7889E-01	0.8114E-01
7	C2H	0.1439E-01	0.1428E-01	0.1419E-01	0.1410E-01	0.1420E-01
8	H2	0.4922E 00	0.4926E 00	0.4923E 00	0.4914E 00	0.4900E 00
9	H	0.6490E-01	0.6612E-01	0.6711E-01	0.6788E-01	0.6871E-01
10	N2	0.3696E-01	0.3668E-01	0.3644E-01	0.3621E-01	0.3599E-01
11	C6H6O	0.6220E-01	0.6106E-01	0.5993E-01	0.5875E-01	0.5751E-01
12	C6H6	0.9056E-02	0.8875E-02	0.8656E-02	0.8385E-02	0.8060E-02
13	NH3	0.7780E-71	0.7720E-71	0.7670E-71	0.7622E-71	0.7576E-71
14	CO	0.1167E 00	0.1165E 00	0.1166E 00	0.1174E 00	0.1183E 00
15	CO2	0.2675E-01	0.2650E-01	0.2625E-01	0.2547E-01	0.2469E-01
16	H2O	0.4620E-04	0.3917E-04	0.3358E-04	0.2896E-04	0.2511E-04
17	OH	0.3785E-01	0.3756E-01	0.3732E-01	0.3709E-01	0.3686E-01
18	O	0.9526E-03	0.9454E-03	0.9530E-03	0.1486E-02	0.2002E-02
19	C	0.7969E 00	0.7911E 00	0.7861E 00	0.7813E 00	0.7767E 00

# INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0019	0.0019	0.0020	0.0020	0.0021
TEMPERATURE (OF)	4702.4	4793.9	4884.4	4974.1	5063.1
PRESSURE (LB/FT2)	2162.2	2162.0	2161.7	2161.5	2161.2
MASS FLUX(LB/FT2-SEC)	0.1684	0.1684	0.1684	0.1685	0.1685

GAS COMPONENT		COMPOSITION (MOLE/MOLE GAS)				
1	CH2	0.3901E-01	0.3870E-01	0.3812E-01	0.3749E-01	0.3681E-01
2	CH3	0.1797E-01	0.1835E-01	0.1856E-01	0.1868E-01	0.1872E-01
3	CH4	0.4816E-02	0.4053E-02	0.3505E-02	0.3020E-02	0.2594E-02
4	C2H6	0.3688E-09	0.2060E-08	0.1336E-08	0.2239E-08	0.1513E-08
5	C2H4	0.1196E-04	0.1053E-04	0.8926E-05	0.7524E-05	0.6251E-05
6	C2H2	0.7816E-01	0.7972E-01	0.7830E-01	0.7638E-01	0.7318E-01
7	C2H	0.1926E-01	0.2017E-01	0.2388E-01	0.2808E-01	0.3345E-01
8	H2	0.4853E 00	0.4760E 00	0.4645E 00	0.4514E 00	0.4378E 00
9	H	0.7459E-01	0.8450E-01	0.9776E-01	0.1129E 00	0.1290E 00
10	N2	0.3559E-01	0.3519E-01	0.3466E-01	0.3409E-01	0.3348E-01
11	C6H6O	0.5595E-01	0.5431E-01	0.5249E-01	0.5057E-01	0.4862E-01
12	C6H6	0.7654E-02	0.7190E-02	0.6664E-02	0.6100E-02	0.5522E-02
13	NH3	0.7490E-71	0.7406E-71	0.7296E-71	0.7175E-71	0.7046E-71
14	CO	0.1189E 00	0.1199E 00	0.1208E 00	0.1217E 00	0.1225E 00
15	CO2	0.2350E-01	0.2204E-01	0.2026E-01	0.1827E-01	0.1613E-01
16	H2O	0.2175E-04	0.1867E-04	0.1594E-04	0.1358E-04	0.1158E-04
17	OH	0.3645E-01	0.3603E-01	0.3551E-01	0.3494E-01	0.3433E-01
18	O	0.2774E-02	0.3794E-02	0.5010E-02	0.6379E-02	0.7841E-02
19	C	0.7680E 00	0.7593E 00	0.7480E 00	0.7354E 00	0.7219E 00

# INDEPTH FLOW ANALYSIS(NON-EQUILIBRIUM FLOW)

CHAR DEPTH (FT)	0.0021	0.0022	0.0022	0.0023	0.0023
TEMPERATURE (OF)	5151.5	5239.3	5326.6	5413.6	5500.1
PRESSURE (LB/FT2)	2161.0	2160.7	2160.5	2160.3	2160.0
MASS FLUX(LB/FT2-SEC)	0.1685	0.1686	0.1687	0.1688	0.1690

## GAS COMPONENT

## COMPOSITION (MOLE/MOLE GAS)

1	CH2	0.3614E-01	0.3542E-01	0.3476E-01	0.3404E-01	0.3321E-01
2	CH3	0.1869E-01	0.1859E-01	0.1847E-01	0.1828E-01	0.1797E-01
3	CH4	0.2231E-02	0.1917E-02	0.1646E-02	0.1419E-02	0.1253E-02
4	C2H6	0.2312E-08	0.1630E-08	0.2305E-08	0.1704E-08	0.1000E-09
5	C2H4	0.5228E-05	0.4313E-05	0.3641E-05	0.2994E-05	0.2438E-05
6	C2H2	0.7054E-01	0.6742E-01	0.6521E-01	0.6137E-01	0.5658E-01
7	C2H	0.3826E-01	0.4330E-01	0.4752E-01	0.5296E-01	0.5877E-01
8	H2	0.4235E 00	0.4074E 00	0.3924E 00	0.3753E 00	0.3540E 00
9	H	0.1457E 00	0.1649E 00	0.1824E 00	0.2032E 00	0.2300E 00
10	N2	0.3286E-01	0.3221E-01	0.3161E-01	0.3095E-01	0.3020E-01
11	C6H60	0.4668E-01	0.4473E-01	0.4289E-01	0.4102E-01	0.3909E-01
12	C6H6	0.4949E-02	0.4394E-02	0.3876E-02	0.3391E-02	0.2943E-02
13	NH3	0.6917E-71	0.6779E-71	0.6653E-71	0.6514E-71	0.6356E-71
14	CO	0.1235E 00	0.1241E 00	0.1248E 00	0.1250E 00	0.1245E 00
15	CO2	0.1394E-01	0.1180E-01	0.9822E-02	0.8022E-02	0.6397E-02
16	H2O	0.9879E-05	0.8391E-05	0.7179E-05	0.6105E-05	0.5121E-05
17	OH	0.3373E-01	0.3310E-01	0.3251E-01	0.3186E-01	0.3111E-01
18	O	0.9345E-02	0.1076E-01	0.1207E-01	0.1317E-01	0.1405E-01
19	C	0.7082E 00	0.6936E 00	0.6800E 00	0.6650E 00	0.6478E 00

## APPENDIX C

### THERMOPHYSICAL PROPERTIES DATA

This appendix contains all the thermodynamic and physical property data used in this research along with the references and methods used to compute the heat capacity, enthalpy, free energy, thermal conductivity and viscosity of gases. In addition, the thermophysical properties required to characterize both the char and the virgin material are also presented. At the end of the chapter, a brief explanation and a typical input of the Thermochemical Generation Program (TGP) is presented. This program was written to develop a uniform thermodynamic data base for converting thermodynamic information from various sources to a convenient polynomial form.

Thermophysical Properties of Gases: The thermodynamic and physical properties data used by the ABLATIN1 and ABLATIN2 systems is presented. The thermodynamic data is presented in table form giving the values of empirical constants for polynomial fit. In this research it was convenient to use the thermodynamic data in functional form. This procedure not only reduced memory space, but in addition, it reduced the need for interpolation between tables of stored values. Coefficient for the polynomial fits have been obtained from numerous sources, mainly from the work of NASA at Lewis (1), Bauer and Duff at Los Alamos

(2), API Project 44 (8) and JANAF (6). The polynomial equations used for the heat capacity is of the form:

$$\frac{C_P^O}{R} = a + bT + cT^2 + dT^3 + eT^4 \quad (C-1)$$

If we define the sensible enthalpy plus the heat of formation at a reference temperature as  $H_{T_R}^O$ , then:

$$H_T^C = \Delta H_{T_R}^O + \int_{T_R}^T C_P^O dT \quad (C-2)$$

Where  $\Delta H_{T_R}^O$  is the heat of formation at the reference temperature  $T_R$ . Substitution of Equation (C-1) into (C-2) and integrating results after some manipulation results in:

$$\frac{H_T^O}{RT} = a + \frac{b}{2} T + \frac{c}{3} T^2 + \frac{d}{4} T^3 + \frac{e}{5} T^4 + \frac{f}{T} \quad (C-3)$$

The definition of absolute entropy is:

$$S_T^O = \int_0^T \frac{C_P^O}{T} dT \quad (C-4)$$

Hence, substituting Equation (C-1) into Equation (C-4) and integrating results after some manipulation:

$$\frac{S_T^O}{R} = a \ln T + bT + \frac{c}{2} T^2 + \frac{d}{3} T^3 + \frac{e}{4} T^4 \quad (C-5)$$

The definition of Standard Molal Free Energy is

as follows:

$$F_T^O = \bar{H}_T^O - TS_T^O \quad (C-6)$$

Substituting the definitions for  $H_T^O$  and  $S_T^O$  in Equation (C-6) results in a polynomial expression for the free energy which is, after dividing by  $RT$ :

$$\frac{\bar{F}_T^O}{RT} = a(1 - \ln T) - \frac{b}{2} T - \frac{c}{6} T^2 - \frac{dT^3}{12} - \frac{eT^4}{20} + \frac{f}{T} - g \quad (C-7)$$

A set of coefficients is presented in Table C-1 for Equations (C-1), (C-3), (C-5) and (C-7). The coefficients presented in Table C-1 are two temperature intervals. A high temperature interval ( $1000^\circ\text{K}$ - $6000^\circ\text{K}$ ) denoted by the letter H and a low temperature interval ( $300^\circ\text{K}$ - $1000^\circ\text{K}$ ) denoted by the letter L. Most of the data used was from McBride et. al. (1) of NASA, covering the intervals  $300^\circ\text{K}$  to  $1000^\circ\text{K}$  and  $1000^\circ\text{K}$  to  $6000^\circ\text{K}$ . At  $1000^\circ\text{K}$  the low and high temperature fits were forced to match. The species for which data of McBride et. al. (1) was used were: C(Graphite), C(g), C<sub>2</sub>, C<sub>3</sub>, CH, CH<sub>2</sub>, CH<sub>3</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, CN, C<sub>2</sub>N<sub>2</sub>, CO, CO<sub>2</sub>, H, H<sub>2</sub>, HCO, H<sub>2</sub>O, N, N<sub>2</sub>, NH, NH<sub>3</sub>, NO, NO<sub>2</sub>, N<sub>2</sub>O, N<sub>2</sub>O<sub>4</sub>, O, O<sub>2</sub> and OH. The coefficients presented for the other species were obtained using the heat capacity coefficients of Duff et. al. (2) and the other two coefficients, f and g, were calculated from them.

TABLE C-1: Coefficients for the Empirical Fit of

$$C_p^o/R, S_T^o/R \text{ and } \bar{F}_T^o/RT$$

		A	B	C	D	E	F	G
C(G)	H	.2579E1	-.1437E-3	.7225E-7	-.7417E-11	.1370E-16	.8543E5	.4321E1
	L	.2541E1	-.2210E-3	.4736E-6	-.4529E-9	.1602E-12	.8545E5	.4573E1
C <sub>2</sub>	H	.4045E1	.1697E-3	.1585E-6	-.5527E-10	.4859E-14	.9961E5	.1281E1
	L	.7509E1	-.1065E-1	.1007E-4	-.8621E-9	-.1752E-11	.9880E5	-.1607E2
C <sub>3</sub>	H	.4713E1	.2903E-2	-.1214E-5	.2285E-9	-.1599E-13	.9375E5	-.2530E1
	L	.2633E1	.9419E-2	-.9593E-5	.5579E-8	-.1424E-11	.9431E5	.8079E1
C <sub>4</sub>	H	.6077E1	.3443E-2	-.9479E-6	.9347E-10	-.1791E-14	.1195E6	-.5995E1
	L	.5670E1	.5883E-2	-.4751E-5	.2349E-8	-.4648E-12	.1195E6	-.4253E1
C <sub>5</sub>	H	.7577E1	.4617E-2	-.1271E-5	.1187E-9	-.1123E-14	.1186E6	-.1431E2
	L	.7279E	.6762E-2	-.5027E-5	.2562E-8	-.5450E-12	.1186E6	-.1311E2
C <sub>6</sub>	H	.9077E1	.5791E-2	-.1595E-5	.1441E-9	-.4628E-15	.1437E6	-.1904E2
	L	.8887E1	.7643E-2	-.5307E-5	.2779E-8	-.6265E-12	.1437E6	-.1837E2
C <sub>7</sub>	H	.1057E2	.6963E-2	-.1917E-5	.1689E-9	.2555E-15	.1435E6	-.2736E2
	L	.1049E2	.8524E-2	-.5585E-5	.2995E-8	-.7075E-12	.1435E6	-.2722E2
C <sub>8</sub>	H	.1207E2	.8133E-2	-.2238E-5	.1934E-9	.9903E-15	.1696E6	-.3209E2
	L	.1211E2	.9403E-2	-.5861E-5	.3207E-8	-.7885E-12	.1696E6	-.3249E2
C <sub>9</sub>	H	.1357E2	.9308E-2	-.2562E-5	.2189E-9	.1641E-14	.1670E6	-.4041E2
	L	.1371E2	.1028E-1	-.6144E-5	.3427E-8	-.8705E-12	.1669E6	-.4134E2
C <sub>10</sub>	H	.1508E2	.1048E-1	-.2885E-5	.2439E-9	.2339E-14	.1966E6	-.4514E2
	L	.1532E2	.1117E-1	-.6421E-5	.3641E-8	-.9510E-12	.1965E5	-.4661E2

		A	B	C	D	E	F	G
CH	H	.1961E1	.3312E-2	-.1469E-5	.2929E-9	-.2124E-13	.7105E5	.1021E2
	L	.3544E1	.8795E-4	-.1826E-5	.4455E-8	-.2186E-11	.7059E5	.1823E1
C <sub>2</sub> H	H	.3513E1	.3589E-2	-.1323E-5	.2305E-9	-.1530E-13	.5789E5	.4523E1
	L	.3006E1	.5537E-2	-.3511E-5	.1249E-8	-.1896E-12	.5797E5	.6920E1
C <sub>3</sub> H	H	.3965E1	.6200E-2	-.2265E-5	.3717E-9	-.2262E-13	.6283E5	.3467E1
	L	.2473E1	.1175E-1	-.8045E-5	.2729E-8	-.3544E-12	.6307E5	.1054E2
C <sub>4</sub> H	H	.5873E1	.7403E-2	-.2729E-5	.4437E-9	-.2637E-13	.7605E5	-.4010E1
	L	.2695E1	.2267E-1	-.2451E-4	.1315E-7	-.2673E-11	.7649E5	.1039E2
C <sub>5</sub> H	H	.5465E1	.1118E-1	-.4299E-5	.7241E-9	-.4441E-13	.9152E5	-.2843E1
	L	.1021E1	.3109E-1	-.3043E-7	.1481E-7	-.2783E-11	.9217E5	.1757E2
C <sub>6</sub> H	H	.8361E1	.1164E-1	-.4637E-5	.8085E-9	-.5150E-13	.1053E6	-.1363E2
	L	.2717E1	.3941E-1	-.4505E-4	.2477E-7	-.5100E-11	.1050E6	.1184E2
C <sub>7</sub> H	H	.9024E1	.1425E-1	-.5733E-5	.1009E-8	-.6475E-13	.1184E6	-.1733E2
	L	.1743E1	.4949E-1	-.5613E-4	.3040E-7	-.6175E-11	.1193E6	.1562E2
C <sub>8</sub> H	H	.9773E1	.1663E-1	-.8198E-5	.1181E-8	-.7600E-13	.1418E6	-.2083E2
	L	.1532E1	.5652E-1	-.6393E-4	.3473E-7	-.7085E-11	.1429E6	.1640E2
C <sub>9</sub> H	H	.1113E2	.1843E-1	-.7453E-5	.1318E-8	-.8510E-13	.1435E6	-.2718E2
	L	.1099E1	.6769E-1	-.7887E-4	.4345E-7	-.8925E-11	.1448E6	.1813E2
C <sub>10</sub> H	H	.1255E2	.2011E-2	-.8136E-5	.1440E-8	-.9305E-13	.1707E6	-.2677E2
	L	.2248E1	.7022E-1	-.8037E-4	.4395E-7	-.9005E-11	.1713E6	.1442E2
CH <sub>2</sub>	H	.2229E1	.4711E-2	-.1766E-5	.3065E-9	-.2017E-13	.3383E5	.7708E1
	L	.3551E1	-.2507E-2	.1235E-4	-.1175E-7	.3812E-11	.3366E5	.1797E1
C <sub>2</sub> H <sub>2</sub>	H	.4497E1	.5269E-2	-.1840E-5	.3105E-9	-.2000E-13	.2563E5	-.3145E1
	L	.7903E0	.2347E-1	-.3554E-4	.2795E-7	-.8448E-11	.2625E5	.1401E2



		A	B	C	D	E	F	G
$C_3H_2$	H	.4501E1	.8696E-2	-.3155E-5	.5242E-9	-.3264E-13	.5191E5	.1827E0
	L	.1668E1	.2219E-1	-.2193E-4	.1110E-7	-.2153E-11	.5230E5	.1305E2
$C_4H_2$	H	.6375E1	.9648E-2	-.3706E-5	.6390E-9	-.4081E-13	.5391E5	-.9060E1
	L	.2071E1	.3115E-1	-.3650E-4	.2047E-7	-.4277E-11	.5449E5	.1033E2
$C_5H_2$	H	.6655E1	.1325E-1	-.5105E-5	.8823E-9	-.5645E-13	.8063E5	-.8785E1
	L	.1006E1	.4108E-1	-.4555E-4	.2475E-7	-.5060E-11	.8139E5	.1669E2
$C_6H_2$	H	.8775E1	.1341E-1	-.5232E-5	.9113E-9	-.5860E-13	.8223E5	-.1805E2
	L	.2324E1	.4629E-1	-.5461E-4	.3087E-7	-.6480E-11	.8307E5	.1082E2
$C_7H_2$	H	.8139E1	.1757E-1	-.6763E-5	.1167E-8	-.7450E-13	.1079E6	-.1389E2
	L	.2029E1	.4775E-1	-.5111E-4	.2777E-7	-.5745E-11	.1088E6	.1366E2
$C_8H_2$	H	.1047E2	.1819E-1	-.7243E-5	.1277E-8	-.8285E-13	.1099E6	-.2657E2
	L	.1087E1	.6487E-1	-.7571E-4	.4207E-7	-.8700E-11	.1112E6	.1567E2
$C_9H_2$	H	.1006E2	.2185E-1	-.8502E-5	.1477E-8	-.9480E-13	.1331E6	-.2275E2
	L	.1691E1	.6335E-1	-.7042E-4	.3834E-7	-.7975E-11	.1342E6	.1499E2
$C_{10}H_2$	H	.1322E2	.2166E-1	-.8660E-5	.1532E-8	-.9955E-13	.1381E6	-.3773E2
	L	.1810E1	.7857E-4	-.9245E-4	.5162E-7	-.1072E-10	.1396E6	.1359E2
$CH_3$	H	.2803E1	.6250E-2	-.2289E-5	.3899E-9	-.2528E-13	.1579E5	.5684E1
	L	.3399E1	.4267E-2	.2033E-6	.1155E-8	.4129E-12	.1565E5	.2703E1
$C_2H_3$	H	.3481E1	.8497E-2	-.3113E-5	.5189E-9	-.3232E-13	.3179E5	.5172E1
	L	.3147E1	.8039E-2	.1453E-6	-.2569E-8	.7908E-12	.3189E5	.7097E1
$C_3H_3$	H	.4658E1	.1051E-1	-.3955E-5	.6723E-9	-.4248E-13	.3667E5	.6294E0
	L	.2588E1	.1891E-1	-.1393E-4	.5541E-8	-.9075E-12	.3699E5	.1031E2
$C_4H_3$	H	.5749E1	.1248E-1	-.4751E-5	.8136E-9	-.5170E-13	.4909E5	-.3429E1
	L	.2636E1	.2633E-1	-.2312E-4	.1093E-7	-.2068E-11	.4955E5	.1091E2
$C_5H_3$	H	.7099E1	.1455E-1	-.5664E-5	.9844E-9	-.6320E-13	.6543E5	-.9039E1
	L	.2649E1	.3462E-1	-.3266E-4	.1601E-7	-.3088E-11	.6608E5	.1139E2

		A	B	C	D	E	F	G
$C_6H_3$	H	.8312E1	.1640E-1	-.6416E-5	.1118E-8	-.7200E-13	.7660E5	-.1357E2
	L	.2926E1	.4064E-1	-.3886E-4	.1907E-7	-.3666E-11	.7738E5	.1117E2
$CH_4$	H	.1180E1	.1095E-1	-.4062E-5	.7137E-9	-.4749E-13	-.9855E4	.1250E2
	L	.4249E1	-.6912E-2	.3160E-4	-.2971E-7	.9510E-11	.1018E5	-.9175E0
$C_2H_4$	H	.3502E1	.1159E-1	-.4474E-5	.7945E-9	-.5323E-13	.4543E4	.2466E1
	L	.1120E1	.1390E-1	.2656E-5	-.1156E-7	.5238E-11	.5332E4	.1583E2
$C_3H_4^{-1}$	H	.4247E1	.1363E-1	-.5114E-5	.8668E-9	-.5465E-13	.2046E5	.1760E1
	L	.2745E1	.1792E-1	-.7243E-5	-.7208E-10	.5918E-12	.2074E5	.9139E1
$C_3H_4^{-2}$	H	.6126E1	.1306E-1	-.5210E-5	.9194E-9	-.5965E-13	.2072E5	-.9286E1
	L	.2496E1	.1839E-1	-.6755E-5	-.8296E-9	.8053E-12	.2159E5	.9894E1
$C_4H_4^{-1}$	H	.5392E1	.1576E-1	-.6028E-5	.1035E-8	-.6590E-13	.3484E5	-.1649E1
	L	.2231E1	.2772E-1	-.1885E-4	.6522E-8	-.8975E-12	.3535E5	.1331E2
$C_4H_4^{-2}$	H	.5088E1	.1614E-1	-.6192E-5	.1065E-8	-.6790E-13	.3289E5	-.1819E1
	L	.2598E1	.2399E-1	-.1215E-4	.2144E-8	.7127E-13	.3334E5	.1028E2
$C_5H_4^{-1}$	H	.7931E1	.1635E-1	-.6293E-5	.1086E-8	-.6935E-13	.4871E5	-.1361E2
	L	.2468E1	.4229E-1	-.4289E-4	.2225E-7	.4450E-11	.4947E5	.1121E2
$C_5H_4^{-2}$	H	.6560E1	.1792E-1	-.6963E-5	.1208E-8	-.7750E-13	.5111E5	-.6448E1
	L	.2010E1	.3603E-1	-.2778E-4	.1096E-7	-.1733E-11	.5183E5	.1491E2
$C_5H_4^{-3}$	H	.6258E1	.1823E-1	-.7078E-5	.1227E-8	-.7870E-13	.4816E5	-.1868E1
	L	.2211E1	.3393E-1	-.2470E-4	.9332E-8	-.1438E-11	.4881E5	.1722E2
$C_6H_4^{-1}$	H	.7080E1	.1962E-1	-.7668E-5	.1336E-8	-.8589E-13	.6279E5	-.1179E2
	L	.2522E1	.4236E-1	-.3545E-4	.1536E-7	-.2672E-11	.6363E5	.1369E2
$C_6H_4^{-2}$	H	.8014E1	.1965E-1	-.7685E-5	.1339E-8	-.8610E-13	.6326E5	-.1236E2
	L	.3073E1	.3951E-1	-.3103E-4	.1269E-7	-.2109E-11	.6403E5	.1080E2

		A	B	C	D	E	F	G
$C_6H_4^{-3}$	H	.5152E1	.2280E-1	-.8996E-5	.1577E-8	-.1018E-12	.5880E5	-.8328E0
	L	.8791E0	.3417E-1	-.1292E-4	-.2030E-8	.1584E-11	.5961E5	.2033E2
$C_3H_5$	H	.4163E1	.1670E-1	-.6328E-5	.1079E-8	-.6880E-13	.1439E5	.7926E1
	L	.3158E1	.1511E-1	.4407E-5	-.9188E-8	.2697E-11	.1468E5	.1374E2
$C_4H_5^{-1}$	H	.4650E1	.1925E-1	-.7335E-5	.1255E-8	-.7970E-13	.3071E5	.3784E1
	L	.3082E1	.2100E-1	-.2637E-5	-.4696E-8	.1634E-11	.3107E5	.1203E2
$C_4H_5^{-2}$	H	.4710E1	.1999E-1	-.7824E-5	.1364E-8	-.8775E-13	.3024E5	.9718E0
	L	.1593E1	.2699E-1	-.7206E-5	-.4060E-8	.1839E-11	.3086E5	.1666E2
$C_2H_6$	H	.1430E1	.1889E-1	-.7044E-5	.1187E-8	-.7445E-13	-.1143E5	.1401E2
	L	.1430E1	.1889E-1	-.7044E-5	.1187E-8	-.7445E-13	-.1143E5	.1401E2
$C_3H_6^{-1}$	H	.2530E1	.2103E-1	-.7953E-5	.1354E-8	-.8565E-13	.8170E3	.1171E2
	L	.3013E1	.1439E-1	.1195E-4	-.1763E-7	.5647E-11	.8268E3	.1022E2
$C_3H_6^{-2}$	H	.2927E1	.2041E-1	-.7676E-5	.9036E-9	-.8230E-13	.5054E4	.6002E1
	L	.1745E1	.1757E-1	.7810E-5	-.1324E-7	.3826E-11	.5422E4	.1302E2
$C_4H_6^{-1}$	H	.4007E1	.2255E-1	-.8552E-5	.1458E-8	-.9235E-13	.1546E5	.4838E1
	L	.3764E1	.1845E-1	.6784E-5	-.1369E-7	.4487E-11	.1560E5	.6898E1
$C_4H_6^{-2}$	H	.3971E1	.2259E-1	.8575E-5	.1464E-8	-.9285E-13	.1774E5	.5946E1
	L	.2437E1	.2913E-1	-.1298E-4	.6525E-9	.8151E-12	.1794E5	.1293E2
$C_4H_6^{-3}$	H	.3258E1	.2349E-1	-.8975E-5	.1539E-8	-.9780E-13	.1127E5	.8230E1
	L	.1310E1	.3537E-1	-.2098E-4	.4492E-8	.2204E-12	.1142E5	.1629E2
$C_4H_6^{-4}$	H	.2782E1	.2591E-1	-.5997E-5	-.4794E-8	.2247E-11	.1757E5	.1191E2
	L	.3991E1	.2286E-1	-.8745E-5	.1501E-8	-.9550E-13	.1736E5	.6002E1
$C_5H_6$	H	.3601E1	.2668E-1	-.1036E-4	.1799E-8	-.1155E-12	.8326E4	.4317E1
	L	.8735E0	.2770E-1	.4256E-5	-.1439E-7	.4465E-11	.8994E4	.1904E2

		A	B	C	D	E	F	G
$C_6H_6$	H	.4619E1	.2881E-1	-.1124E-4	.1957E-8	-.1257E-12	.7391E4	-.1789E1
	L	.3511E0	.3754E-1	-.7947E-5	-.7509E-8	.3038E-11	.8264E4	.1986E2
$C_3H_8$	H	.1291E1	.2775E-1	-.1047E-4	.1780E-8	-.1124E-12	-.1407E5	.1714E2
	L	.2055E1	.2528E-1	-.8879E-8	-.8879E-8	.3198E-11	-.1425E5	.1318E2
$C_4H_8^{-1}$	H	.2473E1	.2980E-1	-.1134E-4	.1940E-8	-.1231E-12	-.2852E4	.1359E2
	L	.3228E1	.1948E-1	.1816E-4	-.2582E-7	.8205E-11	-.2828E4	.1131E2
$C_4H_8^{-2}$	H	.2293E1	.3011E-1	-.1149E-4	.1971E-8	-.1252E-12	-.1973E4	.1510E2
	L	.2773E1	.2733E-1	.1802E-5	-.1306E-7	.4737E-11	-.2083E4	.1274E2
$C_4H_8^{-3}$	H	.2648E1	.2963E-1	-.1127E-4	.1929E-8	-.1224E-12	-.4064E4	.1182E2
	L	.2332E1	.3207E-1	-.9355E-5	-.3009E-8	.1738E-11	-.4086E4	.1285E2
$C_4H_8^{-4}$	H	.2647E1	.2959E-1	-.1125E-4	.1923E-8	-.1219E-12	-.3370E4	.1219E2
	L	.3218E1	.2521E-1	.3948E-5	-.1345E-7	.4555E-11	-.3452E4	.9706E1
$C_4H_8^{-5}$	H	.3216E1	.2940E-1	-.1127E-4	.1939E-8	-.1235E-12	.1076E4	.4977E1
	L	.1990E0	.3516E-1	-.9240E-5	-.3076E-8	.1213E-11	.1711E4	.2040E2
$C_7H_8$	L	-.5417E1	.7735E-1	-.5841E-4	.2372E-7	-.3986E-11	-.1258E4	.4924E2
	L	-.5417E1	.7735E-1	-.5841E-4	.2372E-7	-.3986E-11	-.1258E4	.4924E2
$C_4H_{10}^{-1}$	H	.4285E1	.2841E-1	-.1161E-4	.2081E-8	-.1363E-12	-.1765E5	.4799E1
	L	.3190E1	.2995E-1	.5455E-5	-.1707E-7	.5811E-11	-.1751E5	.9987E1
$C_4H_{10}^{-2}$	H	.4285E1	.2841E-1	-.1161E-4	.2081E-8	-.1363E-12	-.1799E5	.4816E1
	L	.1879E2	-.1312E0	.4290E-3	-.4265E-6	.1373E-9	-.1833E5	-.4601E2
$C_6H_6O$	L	-.3931E1	.6938E-1	-.5210E-4	.1249E-7	.2091E-11	-.1330E5	.4187E2
	L	-.3931E1	.6938E-1	-.5210E-4	.1249E-7	.2091E-11	-.1330E5	.4187E2
CN	H	.3602E1	.3408E-3	.9716E-7	-.1582E-10	-.4142E-15	.4731E5	.3552E1
	L	.3852E1	-.2763E-2	.6857E-5	-.5413E-8	.1490E-11	.4741E5	.2971E1
$C_2N_2$	H	.6502E1	.4053E-2	-.1664E-5	.3094E-9	-.2148E-13	.3490E5	-.9441E1
	L	.3402E1	.1775E-1	-.2686E-4	.2196E-7	-.7087E-11	.3555E5	.5412E1

		A	B	C	D	E	F	G
CO	H	.2951E1	.1552E-2	-.6191E-6	.1135E-9	-.7788E-14	-.1423E5	.6531E1
	L	.3787E1	-.2171E-2	.5075E-5	-.3473E-8	.7721E-12	-.1436E5	.2633E1
CO <sub>2</sub>	H	.4412E1	.3192E-2	-.1298E-5	.2415E-9	-.1674E-13	-.4894E5	-.7287E0
	L	.2170E1	.1037E-1	-.1073E-4	.6345E-8	-.1628E-11	-.4835E5	.1066E2
H	H	.2500E1	.0000E0	.0000E0	.0000E0	.0000E0	.2547E5	-.4600E0
	L	.2500E1	.0000E0	.0000E0	.0000E0	.0000E0	.2547E5	-.4600E0
HCN	H	.3653E1	.3443E-2	-.1258E-5	.2169E-9	-.1430E-13	.1442E5	.2372E1
	L	.2168E1	.1072E-1	-.1508E-4	.1193E-7	-.3700E-11	.1468E5	.9281E1
HCO	H	.3270E1	.3519E-2	-.1377E-5	.2473E-9	-.1673E-13	-.2782E4	.7304E1
	L	.3864E1	-.5370E-3	.6903E-5	-.6645E-8	.2057E-11	-.2799E4	.4897E1
H <sub>2</sub>	H	.3043E1	.6118E-3	-.7399E-8	-.2030E-10	.2459E-14	-.8549E3	-.1648E1
	L	.2846E1	.41932E-2	-.9611E-5	.9512E-8	-.3309E-11	-.9672E3	-.1411E1
H <sub>2</sub> O	H	.2670E1	.3031E-2	-.8535E-6	.1179E-9	-.6197E-14	.2988E5	.6883E1
	L	.4156E1	-.1724E-2	.5698E-5	-.4593E-8	.1423E-11	-.3028E5	-.6861E0
N	H	.2442E1	.1227E-3	-.8499E-7	.2140E-10	-.1251E-14	.5614E5	.4492E1
	L	.2514E1	-.1124E-3	.2964E-6	-.3246E-9	.1259E-12	.5612E5	.4119E1
NH	H	.2727E1	.1419E-2	-.4582E-6	.7555E-10	-.4617E-14	.3892E5	.6044E1
	L	.3454E1	.5280E-3	-.1972E-5	.2957E-8	-.1208E-11	.3867E5	.2010E1
NH <sub>3</sub>	H	.2149E1	.6492E-2	-.2269E-5	.3739E-9	-.2361E-13	-.6402E4	.9238E1
	L	.3771E1	-.4862E-3	.9874E-5	-.9567E-8	.3131E-11	-.6728E4	.1465E1
NO	H	.3152E1	.1406E-2	-.5707E-6	.1062E-9	-.7372E-14	.9852E4	.6944E1
	L	.4146E1	-.4119E-2	.9692E-5	-.7863E-8	.2230E-11	.9744E4	.2569E1
NO <sub>2</sub>	H	.4612E1	.2638E-2	-.1094E-5	.2081E-9	-.1465E-13	.2340E4	.1367E1
	L	.3434E1	.2223E-2	.6714E-5	-.9742E-8	.3721E-11	.2864E4	.8408E1

		A	B	C	D	E	F	G
N <sub>2</sub>	H	.2854E1	.1597E-2	-.6256E-6	.1131E-9	-.7690E-14	-.8901E3	.6390E1
	L	.3691E1	-.1333E-2	.2650E-5	-.9769E-9	-.9977E-13	-.1062E4	.2287E1
N <sub>2</sub> O	H	.4626E1	.3021E-2	-.1215E-5	.2285E-9	-.1585E-13	.8135E4	-.1146E1
	L	.2382E1	.1035E-1	-.1116E-4	.6958E-8	-.1878E-11	.8723E4	.1022E2
N <sub>2</sub> O <sub>4</sub>	H	.1042E1	.6036E-2	-.2583E-5	.4928E-9	-.3478E-13	-.2741E4	-.2582E2
	L	.3165E1	.2719E-1	-.2535E-4	.1099E-7	-.1660E-11	-.7673E3	.1147E2
O	H	.2537E1	-.1842E-4	-.8801E-8	.5964E-11	-.5574E-15	.2923E5	.4946E1
	L	.3021E1	-.2173E-2	.3754E-5	-.2994E-8	.9077E-12	.2913E5	.2646E1
OH	H	.2889E1	.9983E-3	-.2188E-6	.1980E-10	-.3845E-15	.3881E4	.5559E1
	L	.3823E1	-.1118E-2	.1246E-5	-.2104E-9	-.5255E-13	.3585E4	.5825E0
O <sub>2</sub>	H	.3597E1	.7814E-3	-.2238E-6	.4249E-10	-.3346E-14	-.1192E4	.3749E1
	L	.3719E1	-.2516E-2	.8583E-5	-.8299E-8	.2708E-11	-.1057E4	.3908E1

At the end of the appendix a general purpose program is presented that calculates the seven constants, "a" through "g", when the heat capacity at different temperature intervals, the heat of formation, and entropy at 298°K are supplied.

The first card specifies the order of the polynomial of the heat capacity and the number of data points. From the second card on, the heat capacity data with the corresponding temperature in °K are specified. The last card gives the temperature range over which the value of the heat capacity should be calculated and PRINTED out, and the heat of formation and entropy at 298°K which are necessary in the evaluation of the constants.

Gas Phase Physical Properties: The gas phase physical properties required for the solution of the equations of change are the thermal conductivity and the viscosity. The physical property equations are those presented by Sh rwood and Reid (3).

The thermal conductivity of a pure gas is calculated using the equation shown below:

$$k_{gi} = \frac{2.66 \cdot 13 \times 10^{-5} \left( \frac{T}{M_{wi}} \right) (C_{vi} + 4.47)}{\sigma^2 \Omega_v} \quad (C-8)$$

For an ideal gas the heat capacity at constant volume is  $C_{pi} - R$  and the collision diameter,  $\sigma$ , and collision integral,  $\Omega_v$ , are tabulated for individual gas components

in Table C-2 and Table C-3 respectively. The thermal conductivity of the gas mixture is calculated as:

$$\bar{k}_{gi} = \frac{\sum_{i=1}^n x_i k_g}{\sum_{i=1}^n x_i} \quad (C-9)$$

The viscosity of a pure gas is given by a similar equation:

$$\mu_{gi} = \frac{(2.6693 \times 10^{-3}) \cdot (M_{wi} T)^{1/2}}{\sigma^2 \Omega_v} \quad (C-10)$$

The viscosity of the gas mixture is calculated by the equation approximating the Chapman-Enskog Theory:

$$\bar{\mu} = \frac{\sum_{i=1}^n \mu_i}{\left\{ 1 + \sum_{\substack{j=1 \\ j \neq i}}^n \phi_{ij} \left( \eta_j / \eta_i \right) \right\}^{-1}} \quad (C-11)$$

where the parameter,  $\phi_{ij}$ , is calculated by Equation (C-12) below:

$$\phi_{ij} = \left\{ 1 + \left( \mu_i / \mu_j \right)^{1/2} \left( M_{wj} / M_{wi} \right)^{1/4} \right\}^2 \left\{ \sqrt{8} \left( 1 + M_{wi} / M_{wj} \right)^{1/2} \right\}^{-1} \quad (C-12)$$

#### Thermophysical Properties of the Virgin Material and

Char: The thermophysical properties used were those measured by Southern Research Institute (4). Figure C-1 shows the thermal conductivity plot with temperature for 40% nylon, 25% phenolic resin and 35% phenolic microballoon virgin composite. As is shown in the plot the thermal conductivity variation in the temperature range 200°F to 800°F



Table C-2 Lennard-Jones Potentials<sup>(a)</sup>  
and Enthalpy of Formation<sup>(b)</sup> for the Compounds

Component Name	Molecular Weight, $M_{wi}$	Collision Diameter, $\sigma$ A°	Potential Parameter ÷ Boltzmann Constant $E^\circ/k$ , °K	Enthalpy of Formation (290°K) cal/gram mole
CH <sub>4</sub>	16	3.822	136.5	-17889.0
C <sub>2</sub> H <sub>6</sub>	30	4.418	230.0	-20316.6
C <sub>2</sub> H <sub>4</sub>	28	4.232	205.0	12496.0
C <sub>2</sub> H <sub>2</sub>	26	4.221	185.0	54194.0
C <sub>6</sub> H <sub>6</sub>	78	5.270	440.0	19778.8
C <sub>6</sub> H <sub>6</sub> O	94	5.000	400.0	-23500.0
CO <sub>2</sub>	44	3.966	190.0	-94052.0
CO	28	3.590	110.0	-26416.0
H <sub>2</sub>	2	2.986	33.3	0.0
H <sub>2</sub> O	18	2.649	356.0	-57797.9
HCN	27	3.630	569.1	31100.0
NH <sub>3</sub>	17	3.432	312.0	-11040.0
N <sub>2</sub>	28	3.681	91.5	0.0
O <sub>2</sub>	32	3.433	113.0	0.0

(a) Reid, Robert C. and Thomas K. Sherwood, The Properties of Gases and Liquids, 2nd ed., New York: McGraw-Hill, pp. 632-633. (1966).

(b) Perry, John H., ed., Chemical Engineers' Handbook, 3rd ed., New York: McGraw-Hill, 1950, pp. 236-243.

Table C-3 Values of the Collision Integral  
Based on Lennard-Jones Potential for Calculating  
Pure Component Conductivity and Viscosity

$\bar{k}T/E^\circ$	$\Omega_v$	$\bar{k}T/E^\circ$	$\Omega_v$
0.30	2.785	1.30	1.399
0.35	2.628	1.50	1.314
0.40	2.492	1.70	1.248
0.45	2.368	1.90	1.197
0.50	2.257	2.2	1.138
0.55	2.156	2.6	1.081
0.60	2.065	3.2	1.022
0.65	1.982	4.0	0.9700
0.70	1.908	5.0	0.9269
0.75	1.841	7.0	0.8727
0.80	1.780	10.0	0.8242
0.85	1.725	20.0	0.7432
0.90	1.675	40.0	0.6718
0.95	1.587	70.0	0.6194
1.00	1.629	100.0	0.5882
1.10	1.514	200.0	0.5320
1.20	1.452	400.0	0.4811

Reid, Robert C. and Thomas K. Sherwood, The Properties of Gases and Liquids, 2nd ed.,  
New York: McGraw-Hill, 1966, p. 399.

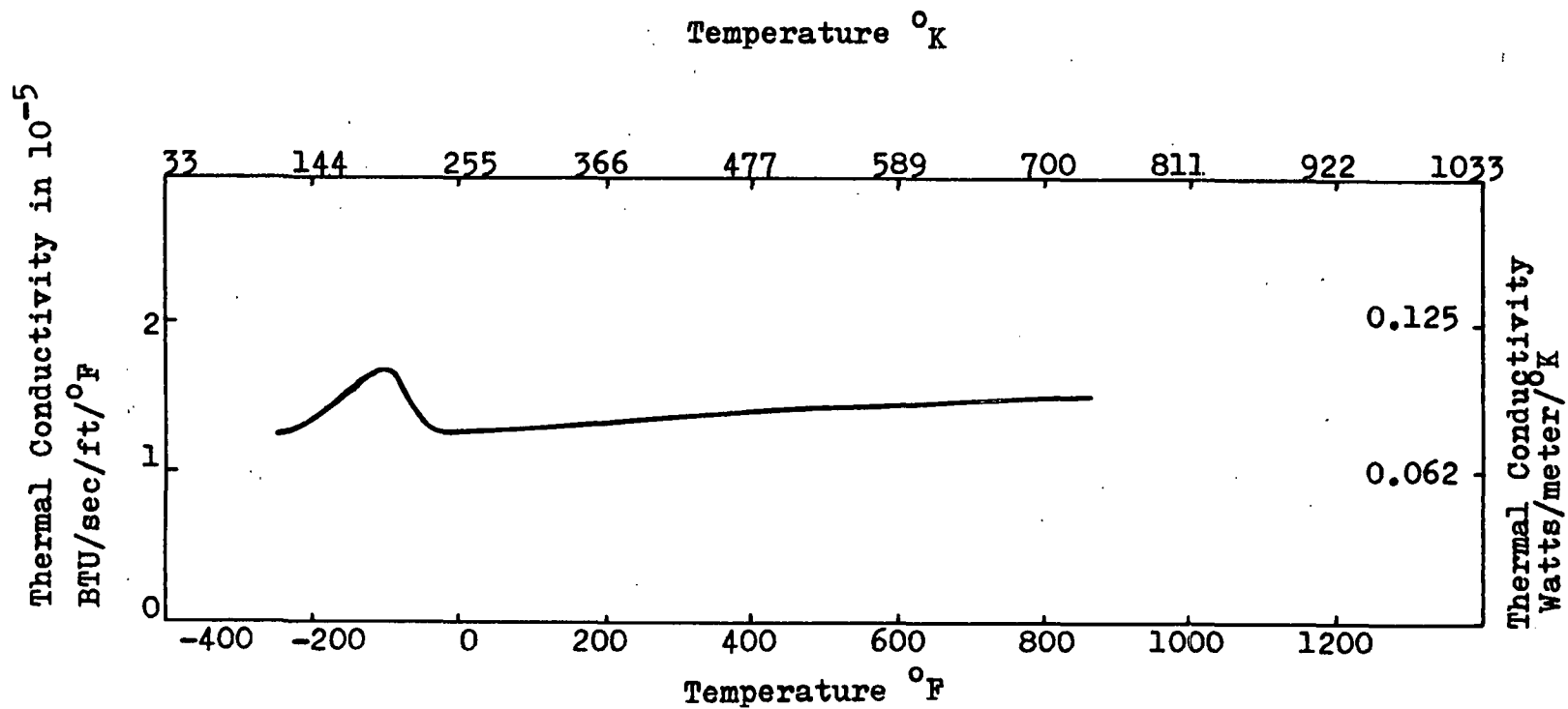


Figure C-1. Thermal Conductivity of Virgin Nylon Phenolic Resin Composite (4).

is small. No further measurements were made beyond 800°F as the degradation of the virgin material made the measurements impractical. However, for the purpose of the computer calculations these measurements were further extrapolated. Figure C-2 shows the thermal conductivity for the low density phenolic nylon char. The thermal conductivity data was fitted empirically by Engelke, et. al. (4) and shown to be:

$$k_e = 11.57 \times 10^{-5} + 5.3 \times 10^{-15} T^3 \quad (C-13)$$

for the temperature range between 800° and 5000°F. The units of  $k_e$  are BTU-ft/sec/ft<sup>2</sup>/°F.

In figure C-3 the heat capacity plot for the virgin material with temperature is shown. A least square fit of this data was performed by Engelke et. al. (4) and was shown to be:

$$C_{P_V} = 0.15 + 4.3 \times 10^{-4} T - 1114 T^{-2} \quad (C-14)$$

where T is the temperature in degrees Rankin.

The heat capacity data for the char was that of Wilson (5) and is shown in Figure C-4.

#### Thermochemical Generation Program

Most of the thermodynamic data available today is usually reported in Table form; be it free energy data, enthalpy data, heat capacity data, entropy, etc. The major sources of such thermodynamic data are reported at the end of the Chapter (1,2,6,8). For an extensive review of other

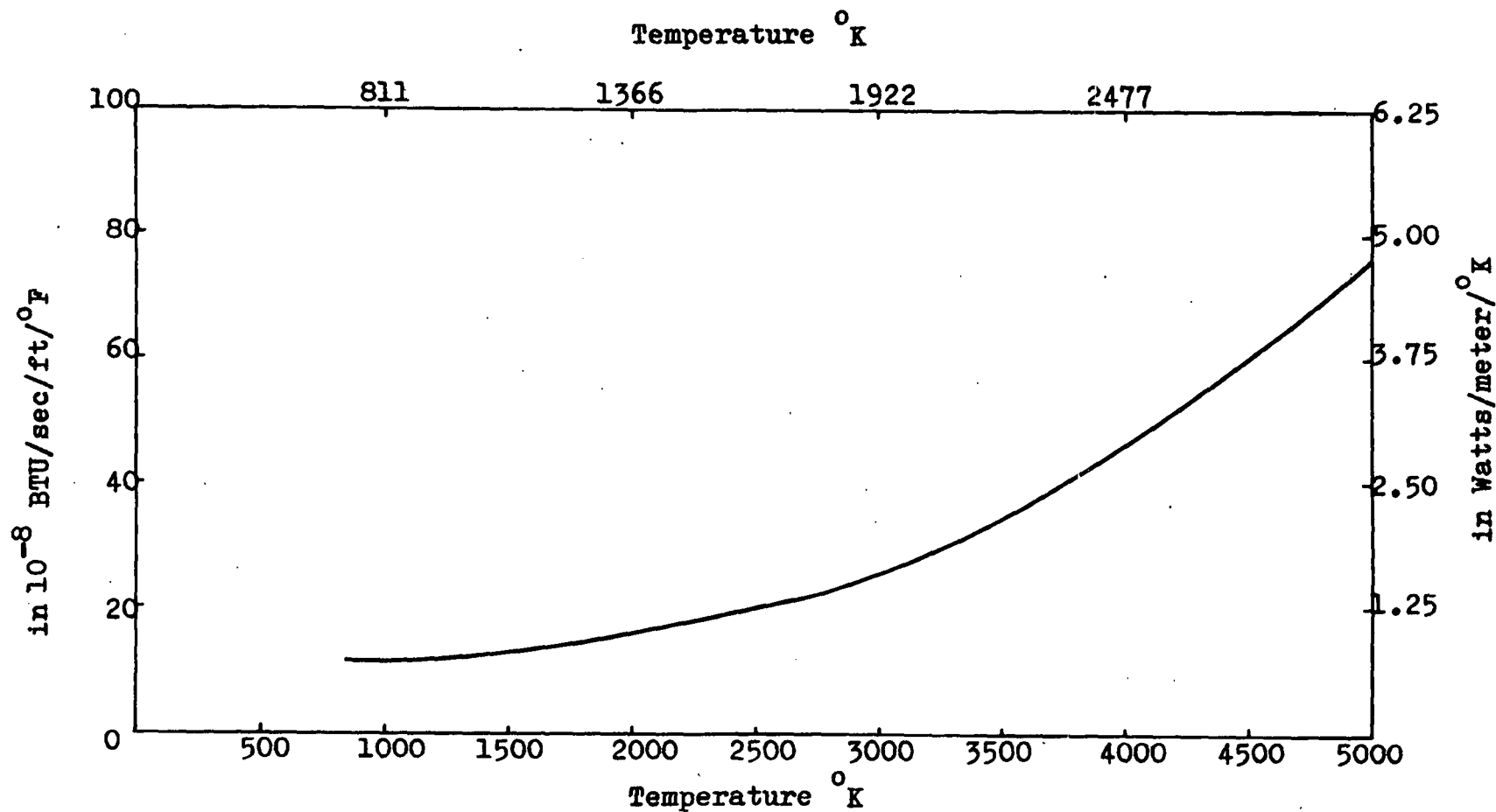


Figure C-2. Thermal Conductivity of Low Density Phenolic Nylon Char (4).

thermodynamic data sources see reference (7).

The thermodynamic data required in the development of both ablating analyses was voluminous. Therefore, to read-in the data in tabular form was ruled out. This would have implied more computer core, and tedious table look up during the computation, which in itself consumes precious computing time. The best alternative, therefore, was to preprocess all the thermodynamic data and reduce them to convenient polynomial forms.

The polynomial forms used for the heat capacity, enthalpy, entropy and free energy data were those published by NASA (1). This format was selected for its convenience and ease of programming. It constituted our initial data base on which we built as our work progressed.

Unfortunately, none of the other major sources of thermodynamic data had reduced them to the convenient polynomial forms of NASA (1). And in these cases where they did (2), the polynomial forms were incompatible with NASA's. It was therefore necessary to develop a Thermochemical Generation Program (TGP) to develop a uniform data base.

The Thermochemical Generation Program (TGP) is a double precision routine that requires heat capacity vs. temperature data, heat of formation at  $298^{\circ}\text{K}$ , and the standard molal entropy at  $298^{\circ}\text{K}$ . With this information TGP proceeds to fit a fourth order polynomial to the heat capacity data as shown in Equation C-1. Once the five constants (a through e) are calculated, the program proceeds

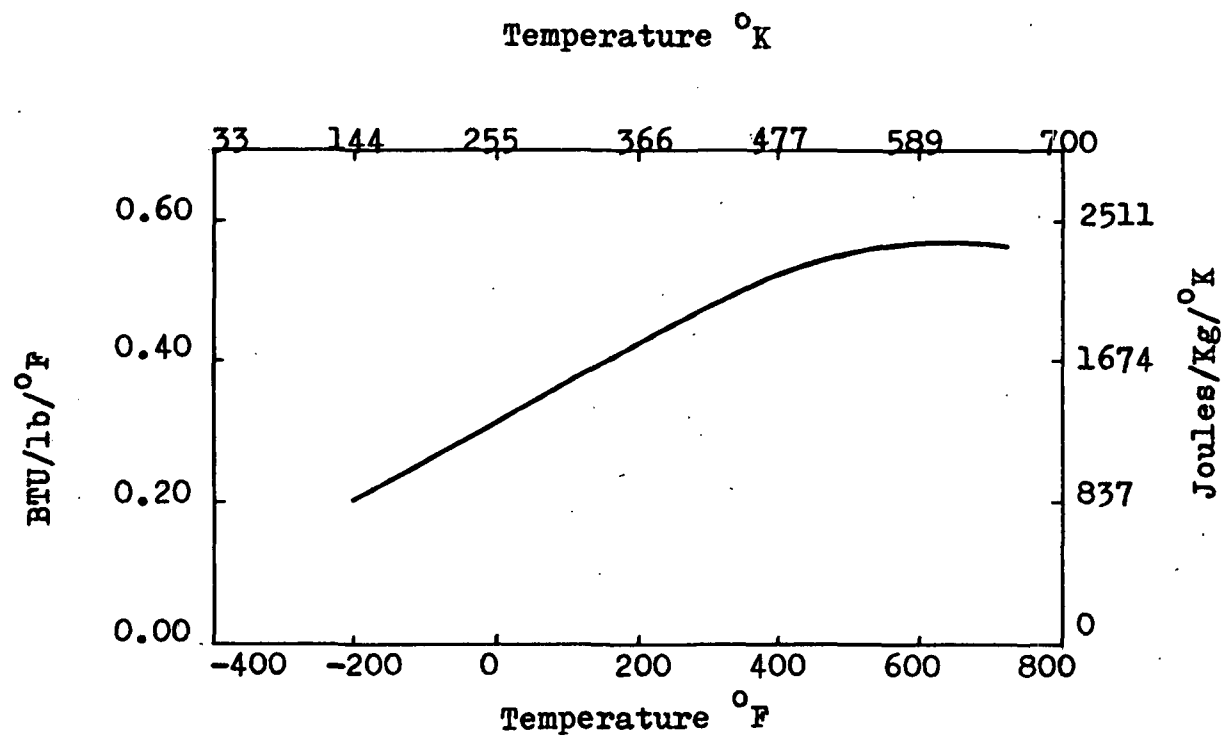


Figure C-3. Heat Capacity of Virgin Material.

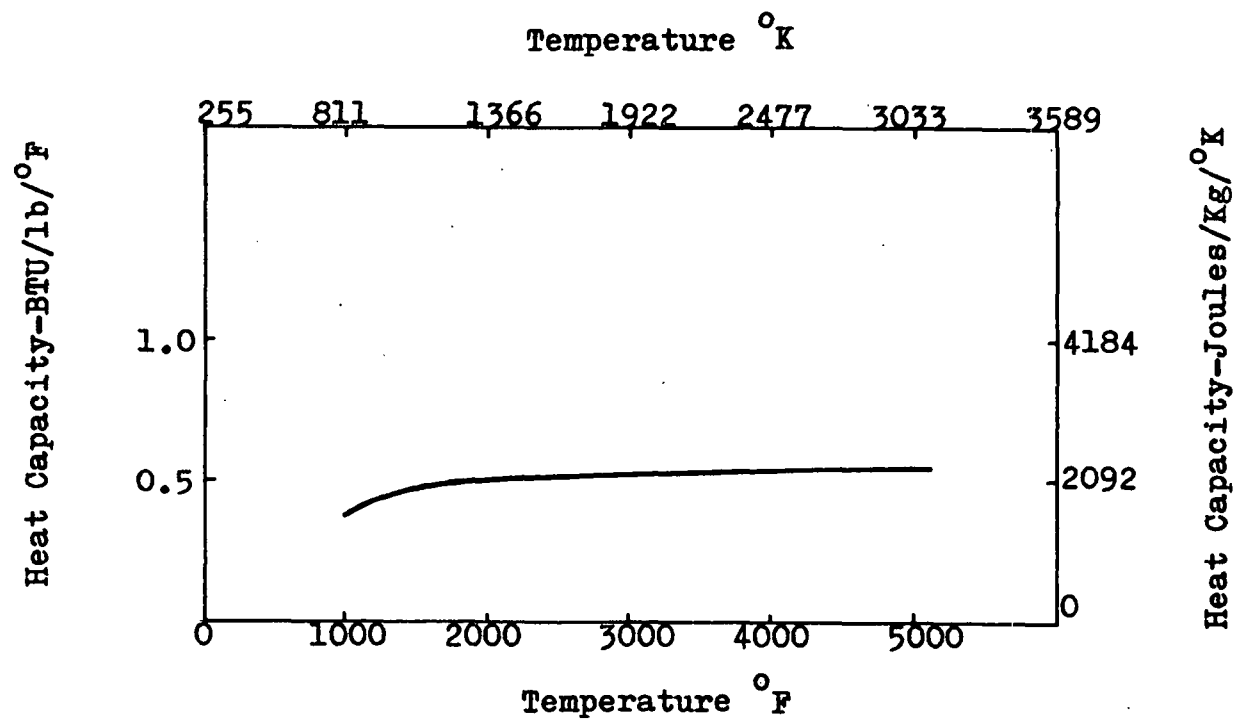


Figure C-4. Heat Capacity of Low Density Phenolic Nylon Char (4).



to compute the constant  $f$  using Equation (C-3) and the known value of the heat of formation at  $298^{\circ}\text{K}$ . Finally, the program calculates the constant  $g$  using Equation (C-5) and the value for the entropy at  $298^{\circ}\text{K}$ . With these seven constants the free energy function could, therefore, be calculated with the use of Equation (C-7). A FORTRAN listing of TGP is presented at the end of the chapter. It is identified by the symbol API44. This was done in honor of API project 44, which was the first concerted effort to develop a consistent set of thermodynamic data for hydrocarbons (8).

TABLE C-4. Listing of Thermochemical Generation Program

	API	1
C	API	2
DOUBLE PRECISION C(7)	API	3
DIMENSION A(7),AP(7)	API	4
C THIS PROGRAM FITS A POLYNOMIAL OF THE FORM A+BT+...+ET(5) TO HEAT	API	5
C CAPACITY DATA USING A LEAST SQUARES DOUBLE PRECISION SUBROUTINE.	API	6
C WITH THESE CONSTANTS IT EVALUATES THE TWO CONSTANTS OF INTEGRATION	API	7
C AP(6) AND AP(7), THAT ARE NECESSARY IN THE EVALUATION OF THE FREE	API	8
C ENERGY FUNCTION FO/RT.THE FORMAT USED FOR THE FREE ENERGY CALCULA-	API	9
C TION IS GIVEN IN NASA SP-3001--THERMODYNAMIC PROPERTIES TO 6000 K	API	10
C FOR 210 SUBSTANCES INVOLVING THE FIRST 18 ELEMENTS--BY B.J.MCBRIDE	API	11
C 1963	API	12
C	API	13
C DELH=HEAT OF FORMATION AT 298 OK	API	14
C S=ABSOLUTE ENTROPY AT 298 OK	API	15
C RR=1.987(UNIVERSAL GAS CONSTANT)	API	16
C TZERO=298.15(BASE TEMPERATURE)	API	17
C FORT=FREE ENERGY	API	18
C CP=HEAT CAPACITY	API	19
C	API	20
RR=1.987	API	21
TZERO=298.15	API	22
TZERO1=TZERO	API	23
TZERO2=TZERO*TZERO1	API	24
TZERO3=TZERO2*TZERO	API	25
TZERO4=TZERO3*TZERO	API	26
TZERO5=TZERO4*TZERO	API	27
C	API	28
C N=TOTAL NUMBER OF CONSTANTS FOR CP POLYNOMIAL	API	29
C	API	30
C CALL THE LEAST SQUARES SUBROUTINE	API	31
C	API	32
100 CALL LSQR(C,N)	API	33
C	API	34

DO 1 I=1,N	API	35
AP(I)=C(I)	API	36
PRINT 101	API	37
101 FORMAT(1H0)	API	38
PRINT 102,AP(I),C(I),I	API	39
102 FORMAT(1X,'AP(I)=' ,E20.8,3X,'HC(I)=' ,D20.9,I6)	API	40
CONTINUE	API	41
READ 2,TINITL,TFINAL,TINC,DELH,S,SNAME	API	42
2 FORMAT(5E10.6,6X,A4)	API	43
PRINT 3, SNAME	API	44
3 FORMAT(//1X,'THE CONSTANTS ARE FOR=' ,A4//)	API	45
C	API	46
C C(I)=POLYNOMIAL CONSTANT	API	47
C	API	48
PRINT 4,TINITL,TFINAL,SNAME,DELH	API	49
4 FORMAT(//1X,9HTINITIAL=,E10.5,3X,'TFINAL='E10.5 ,3X,'HEAT OF FORMAAPI	API	50
ITION OF',A4,1X,'AT 298 OK=' ,E16.5//)	API	51
C CALCULATE HEAT CAPACITY	API	52
T=TINITL	API	53
5 T1=T	API	54
T2=T1*T	API	55
T3=T2*T	API	56
T4=T3*T	API	57
CP=AP(1)+AP(2)*T1+AP(3)*T2+AP(4)*T3+AP(5)*T4	API	58
PRINT 6,CP,T	API	59
6 FORMAT(1X,'CP=' ,E18.5,3X,'T=' ,E18.5)	API	60
T=T+TINC	API	61
IF(T.LE.TFINAL) GO TO 5	API	62
C	API	63
C PROCEED TO CALCULATE THE TWO CONSTANTS OF INTEGRATION AP(6)-AP(7)	API	64
C	API	65
AP(6)=- (AP(1)*TZERO+AP(2)*TZERO2/2.+AP(3)*TZERO3/3.+AP(4)*TZERO4/4API	API	66
1.+AP(5)*TZERO5/5.)	API	67
X=AP(6)	API	68

AP(7)=AP(1)*ALOG(TZERO)+AP(2)*TZERO+AP(3)*TZERO2/2.+AP(4)*TZERO3/3	API	69
1.+AP(5)*TZERO4/4.	API	70
X1=AP(7)	API	71
AP(7)=-X1+S	API	72
PRINT 7,AP(6),AP(7),S	API	73
7 FORMAT (//1X,'AP(6)=' ,E15.5,2X,'AP(7)=' ,E15.5,' S=' ,E15.51)	API	74
AP(6)=X+DELH	API	75
MM=N+2	API	76
DO 8 I=1,MM	API	77
8 A(I)=AP(I)/RR	API	78
PRINT 9,(A(I),I=1,MM)	API	79
9 FORMAT(/1X,7E17.7/)	API	80
C	API	81
C CALCULATE THE FREE ENERGY	API	82
C	API	83
T=TINITL	API	84
10 T1=T	API	85
T2=T1*T	API	86
T3=T2*T	API	87
T4=T3*T	API	88
A2=A(2)	API	89
A1=A(1)	API	90
FORT=A1*(1.-ALOG(T))-A2*T/2.-A(3)*T2/6.-A(4)*T3/12.-A(5)*T4/20.	API	91
1+A(6)/T -A(7)	API	92
PRINT 11,FORT,T	API	93
11 FORMAT(1X,'FORT=' ,E15.5,' T=' ,E15.5)	API	94
T=T + TINC	API	95
IF(T.LE.TFINAL)GO TO 10	API	96
PRINT 13	API	97
13 FORMAT(1H1)	API	98
GO TO 100	API	99
12 STOP	API	100
END	API	101

C	SUBROUTINE LSQR(CC,M,NUMBER,Y,X)	LSQR	1
C		LSQR	2
C		LSQR	3
C	LEAST SQUARE CURVE FITTING OF ANY ORDER POLYNOMIAL	LSQR	4
C	OF ORDER EQUAL TO OR LESS THAN 10	LSQR	5
C		LSQR	6
C		LSQR	7
C		LSQR	8
C	NUMBER IS THE ACTUAL NUMBER OF X-Y DATA PAIRS.,MAXIMUM OF 200	LSQR	9
C	M IS THE DEGREE OF THE POLYNOMIAL.,MAXIMUM OF 10	LSQR	10
C	N IS THE NUMBER OF EQUATIONS(=M+1)	LSQR	11
C	X,Y IS THE ARRAY FOR THE DATA PAIRS	LSQR	12
C	A IS THE ARRAY FOR THE SUM, WHICH BECOME THE COEFFICIENTS OF THE	LSQR	13
C	UNKNOWN IN THE SIMULTANEOUS EQUATIONS.	LSQR	14
C	B IS THE ARRAY FOR THE CONSTANT TERMS IN THE SIMULTANEOUS EQUATION	LSQR	15
C	C IS THE ARRAY FOR THE UNKNOWN, WHICH BECOME THE COEFFICIENS IN	LSQR	16
C	THE POLYNOMIAL.	LSQR	17
C	P IS THE ARRAY FOR THE POWERS OF THE X(I),FROM 1 TO 2M.	LSQR	18
C		LSQR	19
	DOUBLE PRECISION X( 30),Y( 30),A(7,7),B(7),C(7),P(20),TEMP,FACTOR,	LSQR	20
1	SUM	LSQR	21
	DIMENSION CC(3)	LSQR	22
17	READ 20,NUMBER,M	LSQR	23
20	FORMAT(2I6)	LSQR	24
	DO 11 I=1,NUMBER	LSQR	25
	READ 10,Y(I),X(I)	LSQR	26
C	Y(I)=1./Y(I)	LSQR	27
10	FORMAT(2D10.0)	LSQR	28
11	CONTINUE	LSQR	29
	MX2=M*2	LSQR	30
	DO 13 I=1,MX2	LSQR	31
	P(I)=0.0	LSQR	32
	DO 13 J=1,NUMBER	LSQR	33
	POWER=I	LSQR	34

13	P(I)=P(I)+X(J)**POWER	LSQR	35
C		LSQR	36
C		LSQR	37
C	DEVELOPING THE COEFFICIENTS AND THE CONSTANT TERMS OF THE NORMAL	LSQR	38
C	EQUATIONS.	LSQR	39
C		LSQR	40
C		LSQR	41
	N=M+1	LSQR	42
	DO 30 I=1,N	LSQR	43
	DO 30 J=1,N	LSQR	44
	K=I+J-2	LSQR	45
	IF(K)29,29,28	LSQR	46
28	A(I,J)=P(K)	LSQR	47
	GO TO 30	LSQR	48
29	A(1,1)=NUMBER	LSQR	49
30	CONTINUE	LSQR	50
	B(1)=0.	LSQR	51
	DO 21 J=1,NUMBER	LSQR	52
21	B(1)=B(1)+Y(J)	LSQR	53
	DO 22 I=2,N	LSQR	54
	B(I)=0.	LSQR	55
	DO 22 J=1,NUMBER	LSQR	56
22	B(I)=B(I)+Y(J)*X(J)**(I-1)	LSQR	57
C		LSQR	58
C	PIVOTAL CONDENSATION	LSQR	59
C		LSQR	60
	NM1=N-1	LSQR	61
	DO 300 K=1,NM1	LSQR	62
	KP1=K+1	LSQR	63
	L=K	LSQR	64
	DO 400 I=KP1,N	LSQR	65
	IF(DABS(A(I,K))-DABS(A(L,K)))400,400,401	LSQR	66
401	L=I	LSQR	67
400	CONTINUE	LSQR	68

IF(L-K) 500,500,405	LSQR	69
405 DO 410 J=K,N	LSQR	70
TEMP=A(K,J)	LSQR	71
A(K,J)=A(L,J)	LSQR	72
410 A(L,J)=TEMP	LSQR	73
TEMP=B(K)	LSQR	74
B(K)=B(L)	LSQR	75
B(L)=TEMP	LSQR	76
C	LSQR	77
C ELIMINATION, BACK SOLUTION, AND PRINTING RESULTS	LSQR	78
C	LSQR	79
500 DO 300 I=KP1,N	LSQR	80
FACTOR=A(I,K)/A(K,K)	LSQR	81
A(I,K)=0.0	LSQR	82
DO 301 J=KP1,N	LSQR	83
301 A(I,J)=A(I,J)-FACTOR*A(K,J)	LSQR	84
300 B(I)=B(I)-FACTOR*B(K)	LSQR	85
C(N)=B(N)/A(N,N)	LSQR	86
I=NM1	LSQR	87
710 IP1=I+1	LSQR	88
SUM=0.0	LSQR	89
DO 700 J= IP1,N	LSQR	90
700 SUM=SUM+A(I,J)*C(J)	LSQR	91
C(I)=(B(I)-SUM)/A(I,I)	LSQR	92
I=I-1	LSQR	93
IF(I) 800,800,710	LSQR	94
800 DO 900 I=1,N	LSQR	95
CC(I)=C(I)	LSQR	96
900 PRINT 901, I,C(I)	LSQR	97
901 FORMAT(1X,I6,5X,D17.8)	LSQR	98
PRINT 9143	LSQR	99
9143 FORMAT(//T46, 'LINEAR INTERPOLATION', ///T5, 'OBSERVATION',	LSQR	100
1 T27, 'CALCULATION', T49, 'RESIDUAL', T67, 'READING NO.'///)	LSQR	101
DO 905 I=1,NUMBER	LSQR	102

C	XKK=C(1)+C(2)*X(I)+C(3)*X(I)**2	LSQR 103
	XKK=C(1)+C(2)*X(I)	LSQR 104
	RESID = Y(I)- XKK	LSQR 105
C	PRINT 904,XK,X(I)	LSQR 106
	XK=XKK	LSQR 107
	YY = Y(I)	LSQR 108
	XX = X(I)	LSQR 109
	PRINT 904,YY,XK,RESID,XX	LSQR 110
904	FORMAT(4E20.6)	LSQR 111
905	CONTINUE	LSQR 112
902	FORMAT(1H1)	LSQR 113
	RETURN	LSQR 114
	END	LSQR 115



INPUT FORMAT FOR T G P

<u>CARD 1:</u>	<u>FORMAT (2I6)</u>	<u>COLUMNS</u>
NUMBER =	Number of heat capacity data points.	1-6
M =	Order of polynomial fit.	7-12
 <u>CARD 2:</u> <u>FORMAT (2D10.1)</u>		
X(I) =	Heat Capacity data (cal/gm-mole-°K).	1-10
Y(I) =	Temperature (°K).	11-20
 <u>CARD 3:</u> <u>FORMAT (5E10.6, 6x, A4)</u>		
TINITL =	Initial temperature of fit.	1-10
TFINAL =	Final temperature of fit	11-20
TINC =	Increment at which data is to be printed.	21-30
DELH =	Heat of formation of the species at 298°K.	31-40
S =	Entropy at 298°K.	41-50
SNAME =	Species name.	55-60

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## APPENDIX D

## ISOTHERMAL ANALYSIS PROGRAM

This program was developed to study hundreds of possible chemical reactions that could occur in the C-H-O-N system. With this program we were able to determine if reactions were important between the temperature range of 500°K to 3500°K.

The procedure was to use stoichiometric amounts of reactants and calculate the conversion at a given temperature through a char one quarter of an inch thick. This procedure was repeated at higher temperatures and the behavior of the reaction was recorded for later analysis. Those reactions for which the conversions at 3500°K were less than 5 percent were eliminated. It was felt that since the actual char would have an average temperature much less than 3500°K, it was a conservative criteria to select the reaction on this basis.

As it turned out many reactions which had a conversion greater than 5 percent were later eliminated since many of the reactants were present in trace amounts, and therefore, even if their conversion at 3500°K was 100 percent, their contribution to heat absorption was considered negligible. These decisions were based on the composition of gases entering the char. How these compositions were estimated

is explained in Appendix F.

It should be pointed out that the isothermal analysis approach used in this research was different from that used by April (1). April only considered the reactions to be irreversible. In this research, reverse reaction rate constants were used. The reverse reaction rate constants were computed from the known equilibrium constant calculated from the chemical equilibrium program. Table D-1 lists the isothermal analysis program.

TABLE D-1. Listing of the Isothermal Analysis Program

C	CALCULATION OF THE CONVERSION FOR CHEMICAL REACTIONS	ISOT	1
C	THAT POSSIBLY OCCUR IN THE DECOMPOSITION ZONE OF	ISOT	2
C	CHARRING ABLATORS. THE RESULTS COMPUTED ARE FOR THE	ISOT	3
C	ISOTHERMAL FLOW IN THE CHAR ZONE AT TEMPERATURES	ISOT	4
C	FROM 500 OK-3500 OK	ISOT	5
C		ISOT	6
C		ISOT	7
	DIMENSION EQN(18)	ISOT	8
	DOUBLE PRECISION R22,R33,P11,P22,P33,FR1,FR2,FR3,FP1,FP2,FP3,	ISOT	9
A	Z,DELZ,RA,FKK,RKK,FKKK,RKKK,CR1,CR2,CR3,CP1,CP2,CP3,HH,RADELZ,	ISOT	10
B	FT,R44,R55,R66,P44,P55,P66,HMIN,HI,ZZ,ZINC	ISOT	11
	DOUBLE PRECISION TTT	ISOT	12
C		ISOT	13
C	READ THE EQUATION $R1+R2+R3=P1+P2+P3$	ISOT	14
	1111 READ729,(EQN(I),I=1,18)	ISOT	15
	729 FORMAT(18A4)	ISOT	16
C		ISOT	17
C	READ THE STOICHIOMETRIC COEFFICIENTS OF THE RATE EQUATION	ISOT	18
	1112 READ730,R1,R2,R3,P1,P2,P3	ISOT	19
C		ISOT	20
C	READ EXPONENTS ON THE COMPOSITIONS OF THE RATE EQUATION	ISOT	21
	READ 730,R4,R5,R6,P4,P5,P6	ISOT	22
	730 FORMAT(6F4.0)	ISOT	23
C		ISOT	24
C	READ THE MOL WGT OF THE COMPONENTS	ISOT	25
	READ731,FWR1,FWR2,FWR3,FWP1,FWP2,FWP3	ISOT	26
	731 FORMAT(6F5.0)	ISOT	27
C		ISOT	28
C	READ THE INITIAL COMPOSITION OF THE REACTANTS IN MOLE FRACTION	ISOT	29
	READ5,XR1,XR2,XR3,XP1,XP2,XP3	ISOT	30
	5 FORMAT(6E10.0)	ISOT	31
C		ISOT	32
C	READ THE COEFFICIENTS OF THE FORWARD REACTION RATE CONSTANT	ISOT	33
C	UNITS OF AF ARE IN CUBIC-CM,GM-MOLES AND SEC	ISOT	34

C	UNITS OF AEF ARE IN KCAL PER GM-MOLE	ISOT	35
	READ733,AF,SF,AEF	ISOT	36
733	FORMAT(E8.0,2F6.0)	ISOT	37
C		ISOT	38
	READ (5,734 ) A1,A2	ISOT	39
734	FORMAT(1X,2E14.7)	ISOT	40
	READ 735,TINIT,TINC,TFINAL,HI,HMIN	ISOT	41
735	FORMAT(3F10.1,2D10.4)	ISOT	42
	T=TINIT	ISOT	43
C		ISOT	44
828	PRINT829,(EQN(I),I=1,18)	ISOT	45
829	FORMAT(1H1,18A4)	ISOT	46
	PRINT 830	ISOT	47
830	FORMAT( 1X,35HINITIAL COMPOSITION (MOLE FRACTION))	ISOT	48
	PRINT 833,XR1,XR2,XR3,XP1,XP2,XP3	ISOT	49
C		ISOT	50
	PRINT 831	ISOT	51
831	FORMAT(1H0, 'FINAL COMPOSITION (MOLE FRACTION)	ISOT	52
	1 TEMP FRACTIONAL Z DELZ REACTION RATE EK°)	ISOT	53
	PRINT 8311	ISOT	54
8311	FORMAT(1H ,109H R1 R2 R3 P1 P2 P3	ISOT	55
	1 (OF) CONVERSION (MOL/CC-SEC) )	ISOT	56
C		ISOT	57
C	MASS FLUX OF DECOMPOSITION PRODUCTS, W, IN LB/FT2-SEC	ISOT	58
	W=0.01	ISOT	59
C		ISOT	60
C	INITIAL VALUE OF TEMPERATURE,T,IS 500-OK	ISOT	61
	R22=R2/R1	ISOT	62
	R33=R3/R1	ISOT	63
	P11=P1/R1	ISOT	64
	P22=P2/R1	ISOT	65
	P33=P3/R1	ISOT	66
	ZINC=1.D-3	ISOT	67
	R44=R4	ISOT	68

R55=R5	ISOT	69
R66=R6	ISOT	70
P44=P4	ISOT	71
P55=P5	ISOT	72
P66=P6	ISOT	73
DELZ=HI	ISOT	74
C INITIAL VALUE OF THE PRESSURE ,P, IS 1.0 ATMS	ISOT	75
P=1.0	ISOT	76
C GAS CONSTANT,R,IN CALORIES/GMMOLE-OK	ISOT	77
R=1.987	ISOT	78
C	ISOT	79
C CALCULATION OF THE AVERAGE MOL WGT OF THE GAS,FWA	ISOT	80
C ENTERING THE CHAR ZONE	ISOT	81
FWAR=FWR1*XR1+FWR2*XR2+FWR3*XR3	ISOT	82
FWAP=FWP1*XP1+FWP2*XP2+FWP3*XP3	ISOT	83
FWA=FWAR+FWAP	ISOT	84
C	ISOT	85
C CALCULATION OF THE MOLAL FLOW RATE OF THE GAS,FTO	ISOT	86
C FTO HAS UNITS OF GMMOLES PER CM2-SEC	ISOT	87
ACON4=453.59/929.0304	ISOT	88
FTO=W/FWA*ACON4	ISOT	89
C	ISOT	90
C CALCULATION OF MOLAL FLUX OF THE INDIVIDUAL COMPONENTS	ISOT	91
C MOLAL FLUX UNITS ARE GMMOLES PER FT-FT SEC	ISOT	92
FR10=XR1*FTO	ISOT	93
FR20=XR2*FTO	ISOT	94
FR30=XR3*FTO	ISOT	95
FP10=XP1*FTO	ISOT	96
FP20=XP2*FTO	ISOT	97
FP30=XP3*FTO	ISOT	98
C	ISOT	99
C CALCULATION OF THE SPACE TIME,ST,IN CUBIC-CM SEC/GMMOLES	ISOT	100
ST=(0.25*144.0)/(FTO*0.06103)	ISOT	101
C	ISOT	102

C	FT HAS UNITS OF GM-MOLES/CM2-SEC	ISOT 103
	FT=FT0	ISOT 104
2221	FR1=FR10	ISOT 105
	FR2=FR20	ISOT 106
	FR3=FR30	ISOT 107
	FP1=FP10	ISOT 108
	FP2=FP20	ISOT 109
	FP3=FP30	ISOT 110
	ZZ=0.	ISOT 111
	Z=0.	ISOT 112
C		ISOT 113
C	CALCULATION OF THE COMPOSITION OF THE REACTING MIXTURE	ISOT 114
C	C/S ARE CONCENTRATIONS IN GMMOLES/CUBIC-CM	ISOT 115
	RR=82.054	ISOT 116
	TOK=T	ISOT 117
C		ISOT 118
C	CALCULATION OF RATE CONSTANTS FOR FORWARD AND REVERSE REACTIONS	ISOT 119
C	RATE CONSTANT UNITS ARE IN CUBIC CM,GMMOLES AND SEC	ISOT 120
C		ISOT 121
C	FORWARD REACTION RATE CONSTANT, FK	ISOT 122
	FK=AF*TOK**(-SF)*EXP((-AEF*1000.0)/(R*TOK))	ISOT 123
C	REVERSE REACTION RATE CONSTANT, RK	ISOT 124
C		ISOT 125
	EK=EXP(A1+A2/T)	ISOT 126
	COEF=P4+P5+P6-R4-R5-R6	ISOT 127
	EKK=EK/((RR*T)**COEF)	ISOT 128
	RK=FK/EKK	ISOT 129
	FKK=FK	ISOT 130
	RKK=RK	ISOT 131
2222	H=P/(RR*TOK*FT)	ISOT 132
	HH=H	ISOT 133
	CR1=FR1*HH	ISOT 134
	CR2=FR2*HH	ISOT 135
	CR3=FR3*HH	ISOT 136



CP1=FP1*HH	ISOT 137
CP2=FP2*HH	ISOT 138
CP3=FP3*HH	ISOT 139
FKKK=FKK*CR1**R44	ISOT 140
IF(R55.LE.0.) GO TO 520	ISOT 141
FKKK=FKKK*CR2**R55	ISOT 142
IF(R66.LE.0.) GO TO 520	ISOT 143
FKKK=FKKK*CR3**R66	ISOT 144
520 RKKK=RKK*CP1**P44	ISOT 145
IF(P55.LE.0.) GO TO 521	ISOT 146
RKKK=RKKK*CP2**P55	ISOT 147
IF(P66.LE.0.) GO TO 521	ISOT 148
RKKK=RKKK*CP3**P66	ISOT 149
IF(SF.EQ.0.)GOTO521	ISOT 150
TTT=T**(-SF)	ISOT 151
FKKK=FKKK*TTT	ISOT 152
521 RA=FKKK-RKKK	ISOT 153
IF(RA.LT.0.)RA=0.	ISOT 154
IF(RA.LE.0.)GOTO5211	ISOT 155
C	ISOT 156
C	ISOT 157
RADELZ=RA*DELZ	ISOT 158
5210 RADELZ=RA*DELZ	ISOT 159
RATIO=RADELZ/FR1	ISOT 160
IF(RATIO.GT.1.E-7)DELZ=DELZ/4.	ISOT 161
IF(RATIO.GT.1.E-7)GOTO5210	ISOT 162
IF(RATIO.LT.1.E-11)DELZ=DELZ*2.	ISOT 163
IF(DELZ.LE.5.D-7)GOTO5211	ISOT 164
IF(RATIO.LT.1.E-11)GOTO5210	ISOT 165
5211 IF(DELZ.LT.HMIN)DELZ=HMIN	ISOT 166
IF(DELZ.GT.1.E-4)DELZ=1.E-4	ISOT 167
RADELZ=RA*DELZ	ISOT 168
FR1=FR1-RADELZ	ISOT 169
FR2=FR2-RADELZ*R22	ISOT 170

FR3=FR3-RADELZ*R33	ISOT 171
FP1=FP1+RADELZ*P11	ISOT 172
FP2=FP2+RADELZ*P22	ISOT 173
FP3=FP3+RADELZ*P33	ISOT 174
FT=FR1+FR2+FR3+FP1+FP2+FP3	ISOT 175
FTT=FR1*FWR1+FR2*FWR2+FR3*FWR3+FP1*FWP1+FP2*FWP2+FP3*FWP3	ISOT 176
FTT=FTT*2.048172	ISOT 177
Z=Z+DELZ	ISOT 178
IF (FR1.LE.0.)GOTO5240	ISOT 179
IF (ZZ.GT.Z)GOTO2222	ISOT 180
RAA=RA	ISOT 181
FR11=FR1	ISOT 182
XCA=1.-FR11/FR10	ISOT 183
YR1=FR1/FT	ISOT 184
YR2=FR2/FT	ISOT 185
YR3=FR3/FT	ISOT 186
YP1=FP1/FT	ISOT 187
YP2=FP2/FT	ISOT 188
YP3=FP3/FT	ISOT 189
Z2=Z	ISOT 190
DZZZ=DELZ	ISOT 191
PRINT 833,YR1,YR2,YR3,YP1,YP2,YP3,T,XCA,Z2,DZZZ,RAA,EK	ISOT 192
PRINT 522,FKKK,RKKK,FTT	ISOT 193
522 FORMAT(1X'FKKK='D25.16,' RKKK='D25.16,' W='F10.7/)	ISOT 194
ZZ=ZZ+ZINC	ISOT 195
IF (RA.LE.0.)GOTO5240	ISOT 196
IF (Z.LT.0.100)GOTO2222	ISOT 197
C CALCULATION OF FINAL COMPOSITION (MOLE FRACTION)	ISOT 198
5240 YR1=FR1/FT	ISOT 199
YR2=FR2/FT	ISOT 200
YR3=FR3/FT	ISOT 201
YP1=FP1/FT	ISOT 202
YP2=FP2/FT	ISOT 203
YP3=FP3/FT	ISOT 204

RAA=RA	ISOT 205
FR11=FR1	ISOT 206
Z2=Z	ISOT 207
DZZZ=DELZ	ISOT 208
123 PRINT 833,YR1,YR2,YR3,YP1,YP2,YP3,T,XCA,Z2,DZZZ,RAA,EK	ISOT 209
PRINT 522,FKKK,RKKK,FTT	ISOT 210
5220 CONTINUE	ISOT 211
XCA=1.-FR11/FR10	ISOT 212
833 FORMAT(1H0,6F8.4,F9.1,F8.4,2X,4E12.5)	ISOT 213
C	ISOT 214
C READ NEW DATA IF THE CONVERSION IS 100 PERCENT	ISOT 215
C CONVERSION WILL BE 100 PERCENT FOR ALL HIGHER TEMPERATURES	ISOT 216
C	ISOT 217
C THEN REPEAT THE CALCULATIONS AT THE NEW TEMPERATURE	ISOT 218
C	ISOT 219
IF(FR1.LE.0.)GOTO2208	ISOT 220
IF(XCA.LT.0.2)T=T+TINC	ISOT 221
T=T+TINC	ISOT 222
IF(XCA.GT.0.97)GOTO2208	ISOT 223
IF(TINC.GT.0.)GOTO2207	ISOT 224
IF(T.GE.TFINAL)GOTO2221	ISOT 225
GOTO2208	ISOT 226
2207 IF(T.LE.TFINAL)GOTO2221	ISOT 227
C	ISOT 228
C RE-INITIALIZE	ISOT 229
C	ISOT 230
C	ISOT 231
2208 PRINT 833,YR1,YR2,YR3,YP1,YP2,YP3,T,XCA,Z2,DZZZ,RAA,EK	ISOT 232
C PRINT DATA	ISOT 233
PRINT 2209,FTT	ISOT 234
2209 FORMAT(1H0,25H MASS FLUX(LB/FT2-SEC) = , F8.4)	ISOT 235
PRINT2210,AF,SF,AEF	ISOT 236
2210 FORMAT(1H0,3HAF=,E9.2,5H SF=,F6.2,6H AEF=,F6.1)	ISOT 237
PRINT2211,AR,SR,AER	ISOT 238

2211	FORMAT(1H0,3HAR=,E9.2,5H SR=,F6.2,6H AER=,F6.1)	ISOT 239
	PRINT2212	ISOT 240
2212	FORMAT(1H0,29HFWR1 FWR2 FWR3 FWP1 FWP2 FWP3)	ISOT 241
	PRINT2213,FWR1,FWR2,FWR3,FWP1,FWP2,FWP3	ISOT 242
2213	FORMAT(1X,6F6.1)	ISOT 243
	PRINT 2218	ISOT 244
2218	FORMAT(1H0,28H STOICHIOMETRIC COEFFICIENTS)	ISOT 245
	PRINT2214	ISOT 246
2214	FORMAT(1H0,24H R1 R2 R3 P1 P2 P3)	ISOT 247
	PRINT2215,R1,R2,R3,P1,P2,P3	ISOT 248
2215	FORMAT(1X,6F4.1)	ISOT 249
	PRINT 2219	ISOT 250
2219	FORMAT(1H0,45H EXPONENTS ON THE COMP. OF THE RATE EQUATION)	ISOT 251
	PRINT 2216	ISOT 252
2216	FORMAT(1H0,24H R4 R5 R6 P4 P5 P6)	ISOT 253
	PRINT 2217,R4,R5,R6,P4,P5,P6	ISOT 254
2217	FORMAT(1X,6F4.1)	ISOT 255
C	READ IN NEW DATA FOR CALCULATIONS OF NEXT EQUATION	ISOT 256
	GOTO1111	ISOT 257
24	STOP	ISOT 258
	END	ISOT 259

INPUT FORMAT FOR THE ISOTHERMAL ANALYSIS PROGRAM

CARD 1:      FORMAT (18A4)                      COLUMNS

EQN(I) = Alphameric Reaction Expression      1-72

CARD 2:      FORMAT (6F4.0)

R1 = Stoichiometric coefficient of  
Reactant 1                                      1-4

R2 = Stoichiometric Coefficient of  
Reactant 2                                      5-8

R3 = Stoichiometric Coefficient of  
Reactant 3                                      9-12

P1 = Stoichiometric Coefficient of  
Product 1                                      13-16

P2 = Stoichiometric Coefficient of  
Product 2                                      17-20

P3 = Stoichiometric Coefficient of  
Product 3                                      21-24

CARD 3:      FORMAT (6F4.0)

R4 = Exponent of Reactant 1                      1-4

R5 = Exponent of Reactant 2                      5-8

R6 = Exponent of Reactant 3                      9-12

P4 = Exponent of Product 1                      13-16

P5 = Exponent of Product 2                      17-20

P6 = Exponent of Product 3                      21-24

CARD 4:      FORMAT (6F5.0)

FWR1 = Molecular Weight of Reactant 1      1-5

FWR2 = Molecular Weight of Reactant 2      6-10

FWR3 = Molecular Weight of Reactant 3      11-15

COLUMNS

FWP1 = Molecular Weight of Product 1	16-20
FWP2 = Molecular Weight of Product 2	21-25
FWP3 = Molecular Weight of Product 3	26-30

CARD 5:   FORMAT (3E10.0)

XR1 = Mole Fraction of Reactant 1	1-10
XR2 = Mole Fraction of Reactant 2	11-20
XR3 = Mole Fraction of Reactant 3	21-30

CARD 6:   FORMAT (E8.0, 2F6.0)

AF = Frequency Factor ( $\text{cm}^3/\text{gm-mole/sec}$ )	1-8
SF = Exponent on Temperature	9-14
AEF = Activation Energy ( $\text{Kcal/gm-mole}$ )	15-20

CARD 7:   FORMAT (1X, 2E 14.7)

A1 = 1st Constant of Equilibrium Constant	2-15
A2 = 2nd Constant of Equilibrium Constant	16-29

CARD 7 read the constants for the equilibrium constant  
fit of the form  $\text{EXP}(A1+A2/T)$ .

CARD 8:   FORMAT (3F10.1, 2010.4)

TINIT = Initial Temperature ( $^{\circ}\text{K}$ )	1-10
TINC = Temperature Increment ( $^{\circ}\text{K}$ )	11-20
TFINAL = Final Temperature ( $^{\circ}\text{K}$ )	21-30
HI = Initial Step Size (FT)	31-40
HMIN = Minimum Step Size (FT)	41-50

## APPENDIX E

### A DESCRIPTION OF THE CHEMICAL EQUILIBRIUM ANALYSIS PROGRAM

The chemical equilibrium analysis program is based on the free energy minimization method that is described in detail in Chapter IV. This analysis is a general method to calculate the equilibrium composition of a multi-component, polyphase system.

As input, the program requires that the user specify the temperature, pressure and an estimate of the composition of the chemical species of interest which are consistent with the elemental composition. In its present form the program reads in the thermodynamic data as seven constants for a polynomial of the form of Equation (C-7). This method of reading the data into the program is compact and flexible. A brief description of the program follows:

#### The Chemical Equilibrium Analysis Program

The Chemical Equilibrium Program consists of a MAIN executive program and four subroutines. These subroutines are THERMO, HOLD1, TRACE, and MATINV, and a description of each is given in this section.

MAIN: This is the executive routine of the chemical equilibrium program. This program generates the matrix necessary to solve the set of algebraic equations.

These coefficients are calculated following the same procedure described in Chapter IV. The coefficients are those shown in Table 4-1. The MAIN program calls THERMO to get the free energy function, and MATINV to invert the matrix and calculate the Lagrange multipliers. These multipliers are used to re-estimate the values of the composition of the gases for the next iteration as is shown in Equation (4-32). It should be noted, however, that values of  $\chi_i$  are re-adjusted using the convergence procedure described in Chapter IV. This is to avoid possible divergence of the solution. It should be noted also that the composition of the solid species are explicitly solved in the matrix inversion subroutine and are also corrected by the same technique.

THERMO: This subroutine provides the main program with the values of the free energy function for each of the species being calculated. In addition, the program calculates the heat of formation of each species along with the sensible enthalpy change per mole.

The THERMO subroutine uses a polynomial expression similar to the one shown in Equation (C-7) of Appendix C to calculate the free energy function. This polynomial form is a very convenient and efficient way for repetitive calculation. It is certainly more accurate and less time consuming than a table look-up and requires less storage than the table form.



MATINV: This subroutine is a standard method for solving a set of linear equations by inverting a non-singular nxn matrix. The inversion is performed iteratively by reducing the original matrix by a series of row operations. The method is then repeated with the resulting identity matrix. This subroutine is the same as used in the ABLATIN2 analysis that is described in Appendix A.

HOLD1: One of the major numerical drawbacks of the free energy minimization technique is that its convergence speed is reduced quite drastically by the presence of trace species during the numerical calculations. These trace species are those whose composition are less than  $10^{-8}$  and therefore their contribution to the total free energy of the system is computationally negligible.

This subroutine checks for the presence of trace species. This is done if the procedure has not converged within a preset number of iterations. In our case, this number is ten. After checking for trace species, the subroutine re-orders the species in descending order of compositions and eliminates those less than  $10^{-8}$ . However, the program holds the species in storage for a final check at the end of the minimization procedure. This check is performed by subroutine TRACE which is described below.

TRACE: If species have been eliminated during the computational procedure, subroutine TRACE is called to recompute their value at the end of the convergence procedure. The technique used is thoroughly explained in

Chapter IV. The equation used to calculate the trace species is Equation (4-46). A listing of the program follows.

At the end of the Appendix, an example illustrates how to use the program. The example selected is for silicone elastomers, and typical results are presented.

TABLE E-1. Listing of the Chemical Equilibrium Program

C		CHEM	1
C		CHEM	2
C	-----THIS PROGRAM COMPUTES COMPLEX CHEMICAL EQUILIBRIUM FOR	CHEM	3
C	A MULTICOMPONENT, POLYPHASE SYSTEM BY FREE ENERGY MINI-	CHEM	4
C	MIZATION. (J.CHEM.PHYS., VOL28, NO.5, 1958)	CHEM	5
C		CHEM	6
C		CHEM	7
C		CHEM	8
	COMMON/KA/ICODE(40),SPCIE1(40),SPCIE2(40),AA(40,5),	CHEM	9
1	ENT1(40),ENT(40)	CHEM	10
	COMMON/KB/AI(40),BI(40),CI(40),DI(40),EI(40),FI(40);	CHEM	11
1	GI(40),AII(40),BII(40),CII(40),DII(40),EII(40),	CHEM	12
2	FII(40),GII(40),DELH(40),FORT(40),C(40),TLOW(40),	CHEM	13
3	Y(40),XMW(40),MLFRC(40)	CHEM	14
	COMMON/KBB/CPDT1(5),PERC(40),PERC1(40)	CHEM	15
	COMMON/KC/IICODE(40),XPCIE1(40),XPCIE2(40),XAA(40,5),	CHEM	16
1	XENT(40),XENT1(40)	CHEM	17
	COMMON/KD/XAI(40),XBI(40),XCI(40),XDI(40),XEI(40),	CHEM	18
1	XFI(40),XGI(40),XAI1(40),XBII(40),XCI1(40),	CHEM	19
2	XDII(40),XEII(40),XFII(40),XGII(40),XMLFR(40)	CHEM	20
	COMMON/KDD/XDELH(40),XCPDT(40),XCPDT1(05),XFORT(40),	CHEM	21
	1XY(40),XC(40),XTLOW(40),XXMW(40),XPERC(40),XPERC1(40)	CHEM	22
	COMMON/KE/S1(5),S2(5),S3(5),S4(5),S5(5),A11(5),A22(5),	CHEM	23
1	A33(5),A44(5),A55(5),S6(5),A66(5),JCODE(5),S(40)	CHEM	24
	COMMON/KF/NC,NS,MM,RR,MM1,NQ,NN,KW,IN,KOUT,KCODE,KSQID	CHEM	25
	COMMON/KG/T,TZERO,TZERO1,TZERO2,TZERO3,TZERO4,TZERO5,P	CHEM	26
	DIMENSION YSUM(40),XMASS(40),DELT(40),X(40),XLAM(40),	CHEM	27
1	FY(40),R(7,7),B(7,1),PI(7),BB(7),FSUM(40),	CHEM	28
2	XMER(40),YX(40)	CHEM	29
	DIMENSION AAA(40)	CHEM	30
	DIMENSION XMOL(40)	CHEM	31
	DIMENSION XMAS1(20)	CHEM	32
	DIMENSION XMASSS(30)	CHEM	33
	REAL MLFRC	CHEM	34

5	MAXNT=100	CHEM	35
	KX=0	CHEM	36
	KPASSS=0	CHEM	37
	MA=1	CHEM	38
C		CHEM	39
	KSOLID=0	CHEM	40
C		CHEM	41
C	-----READ INITIAL,FINAL,INCREMENTAL AND BASE TEMPERATURE. ALSO READ CR	CHEM	42
C	FOR CONVERGENCE,NUMBER OF GAS AND SOLID SPECIES,AND NUMBER OF ELEM	CHEM	43
C		CHEM	44
C		CHEM	45
C	-----READ INPUT PARAMETERS	CHEM	46
C		CHEM	47
C		CHEM	48
	READ1,XT,TMAX,TINC,TZERO,CRIT,NC,MM,NNS	CHEM	49
	IF(XT.LT.1.)GOTO333	CHEM	50
	NS=NC+NNS	CHEM	51
1	FORMAT(5F10.4,3I6)	CHEM	52
	MMI=MM	CHEM	53
	READ 2,IHCODE,H,IPUNCH	CHEM	54
2	FORMAT(I6,1F10.5,I3)	CHEM	55
C		CHEM	56
C		CHEM	57
C	-----COMPUTE THE SIZE OF THE MATRIX	CHEM	58
C		CHEM	59
C		CHEM	60
	NA=MM+1+NS-NC+IHCODE	CHEM	61
C		CHEM	62
C	NA=SIZE OF MATRIX. IT VARIES WITH THE NUMBER OF ELEMENTS	CHEM	63
C	AND THE NUMBER OF SOLIDS PRESENT IN THE SYSTEM.	CHEM	64
C		CHEM	65
	DO 209 J=1,MM	CHEM	66
C		CHEM	67
C		CHEM	68

C		CHEM	69
C	----READ IN EMPIRICAL CONSTANTS FOR THE ENTHALPY FIT OF THE	CHEM	70
C	ELEMENTS.	CHEM	71
C		CHEM	72
C		CHEM	73
C	S1 THRU S5=EMPIRICAL CONSTANTS FOR HEAT CAPACITY OF ELEMENTS	CHEM	74
C	(ABOVE 1000 OK)	CHEM	75
C	A11 THRU A55=EMPIRICAL CONSTANTS FOR HEAT CAPACITY OF ELEMENTS	CHEM	76
C	(UP TO 1000 OK)	CHEM	77
C		CHEM	78
	READ2111,S1(J),S2(J),S3(J),S4(J),S5(J),S6(J),JCODE(J)	CHEM	79
	2111 FORMAT(6E10.4,I3)	CHEM	80
	210 FORMAT(7E10.8)	CHEM	81
C		CHEM	82
	READ 210,A11(J),A22(J),A33(J),A44(J),A55(J),A66(J)	CHEM	83
	209 CONTINUE	CHEM	84
C		CHEM	85
C		CHEM	86
C	NC IS THE TOTAL NUMBER OF MOLES OF GASES USED IN THE ORIGINAL INPUT	CHEM	87
C	NN WILL DIFFER FROM NC ONLY WHEN TRACE SPECIES ARE ELIMINATED FROM	CHEM	88
C	THE COMPUTATIONS WHILE BEING HELD IN A TEMPORARY LOCATION UNTIL WE	CHEM	89
C	ARE REASONABLY SURE THAT WE ARE VERY CLOSE TO THE MINIMUM.	CHEM	90
C	NS IS THE TOTAL NUMBER OF MOLES OF GASES + SOLIDS BEING READ IN.	CHEM	91
C	IT WILL DIFFER FROM NQ ONLY WHEN TRACE SPECIES APPEAR.	CHEM	92
C		CHEM	93
C		CHEM	94
	KREAD=0	CHEM	95
	NQ=NS	CHEM	96
	NN=NC	CHEM	97
C		CHEM	98
C		CHEM	99
C	-----READ MOLECULAR WEIGHT,INITIAL GUESS,NAME OF SPECIE,AND CODE	CHEM	100
C	TO DETERMINE WETHER THE SPECIE IS ASOLID OR A GAS	CHEM	101
C		CHEM	102

C		CHEM 103
C	NC=NO. OF GAS COMPONENTS	CHEM 104
C	NS=NO. OF CONDENSED PLUS GAS COMPONENTS	CHEM 105
C	MM=NO. OF ELEMENTS	CHEM 106
C	TZERO=REFERENCE TEMPERATURE (298.15 OK)	CHEM 107
C	RR=1.98726(CAL/GM-MOLE-OK)	CHEM 108
C	ICODE=0 (GAS), =1 (SOLID)	CHEM 109
C	SPCIE1 AND SPCIE2 ARE THE SPECIES IDENTIFICATION NAME	CHEM 110
C		CHEM 111
	DO 212 I=1,NS	CHEM 112
	READ 208,TLOW(I),XMW(I),Y(I),SPCIE1(I),SPCIE2(I),	CHEM 113
	1 ICODE(I)	CHEM 114
	208 FORMAT(10X,3E10.4,2X,2A3,I4)	CHEM 115
C		CHEM 116
C		CHEM 117
C	-----READ IN EMPIRICAL CONSTANTS FOR THE ENTHALPY,FREE ENERGY	CHEM 118
C	AND ENTROPY FIT OF THE CHEMICAL SPECIES.	CHEM 119
C		CHEM 120
C		CHEM 121
C		CHEM 122
C	AI THRU GI=EMPIRICAL CONSTANTS FOR HEAT CAPACITY (ABOVE 1000 OK)	CHEM 123
C		CHEM 124
	READ 210, AI(I),BI(I),CI(I),DI(I),EI(I),FI(I),GI(I)	CHEM 125
C		CHEM 126
C	AII THRU GII=EMPIRICAL CONSTANTS FOR HEAT CAPACITY (UP TO 1000 OK)	CHEM 127
C		CHEM 128
	READ 210,AII(I),BII(I),CII(I),DII(I),EII(I),FII(I),GII(I)	CHEM 129
C		CHEM 130
C		CHEM 131
C	-----READ IN THE FORMULA NUMBER	CHEM 132
C		CHEM 133
C		CHEM 134
C		CHEM 135
C	AA(I,J)=FORMULA NUMBER. IT GIVES THE GRAM ATOMS OF ELEMENT	CHEM 136

C	J IN SPECIE I.	CHEM 137
C	READ 210,(AA(I,J),J=1,MM)	CHEM 138
	212 CONTINUE	CHEM 139
C		CHEM 140
C	-----READ THE PRESSURE OF THE SYSTEM.	CHEM 141
C		CHEM 142
	READ3,RR,P	CHEM 143
	3 FORMAT(2F14.8)	CHEM 144
C		CHEM 145
C		CHEM 146
C	-----READ IN THE NUMBER OF ITERATIONS AFTER WHICH TRACE SPECIES	CHEM 147
C	SHOULD BE CHECKED.	CHEM 148
C		CHEM 149
C		CHEM 150
	READ6,NFREQ	CHEM 151
	6 FORMAT(3I6)	CHEM 152
C		CHEM 153
C	CRIT=CRITERIA FOR CONVERGENCE.	CHEM 154
C		CHEM 155
	XBETA=CRIT	CHEM 156
	KSEND=0	CHEM 157
	KSEND1=0	CHEM 158
	KORE=0	CHEM 159
	KOUT=0	CHEM 160
	BETA=0.	CHEM 161
	T=XT	CHEM 162
	KCODE=0	CHEM 163
	LL=NN+1	CHEM 164
C		CHEM 165
C		CHEM 166
C	MLFRC=MOLE FRACTION(INCLUDING SOLIDS)	CHEM 167
C		CHEM 168
	SUM=0.	CHEM 169
		CHEM 170

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      DO 434 I=1,NQ
434  SUM=SUM+Y(I)
C
C-----CALCULATE THE GRAM-ATOMS OF EACH ELEMENT. THIS IS THE
C      MATERIAL BALANCE CONSTRAINT ON THE FREE ENERGY EQUATION
C      BB(J) WILL STAY CONSTANT THROUGHOUT THE CALCULATIONS. VALUES
C      OF Y(I) SHOULD BE IN STOICHIOMETRIC PROPORTION.
C
C
C      BB(J)=GRAM ATOMS OF EACH ELEMENT
C
C
      DO 320 J=1,MM
      BB(J)=0.0
      DO 320 I=1,NQ
      BB(J)=BB(J)+AA(I,J)*Y(I)
320  CONTINUE
C
C
C-----CHECK TO DETERMINE IF THERE ARE ANY SOLIDS IN THE SYSTEM.
C
C
      DO 433 I=1,NQ
      IF(ICODE(I).EQ.0)GOTO433
      KCODE=1
433  CONTINUE
C
C
C-----IF THERE IS NOT AN ENERGY CONSTRAINT GO TO 500.
C
C
      IF(IHCODE.EQ.0)GOTO500
      MM=MM+1
      BB(MM)=H/SUM

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CHEM 203
CHEM 204

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500 PRINT4	CHEM 205
4 FORMAT(1H1,18X,5HFO/RT,11X,12HINITIAL Y(I))	CHEM 206
KX=0	CHEM 207
CALL THERMO	CHEM 208
C	CHEM 209
C	CHEM 210
C-----THERMO SUBROUTINE CALCULATES THE FREE ENRGY FUNCION,THE HEAT OF	CHEM 211
C FORMATION OF EVERY CHEMICAL SPECIE AT ANY TEMPERATURE T,AND THE	CHEM 212
C SENSIBLE ENTHALPY CHANGE PER MOLE OF EACH SPECIE.	CHEM 213
C	CHEM 214
C	CHEM 215
DO 206 I=1,NQ	CHEM 216
PRINT 14,I,SPCIE1(I),SPCIE2(I),FORT(I),Y(I)	CHEM 217
14 FORMAT(1X,I3,1X,2A3,2E18.7)	CHEM 218
206 CONTINUE	CHEM 219
45 NTEST=NFREQ	CHEM 220
NT=1	CHEM 221
C	CHEM 222
C	CHEM 223
C-----BETWEEN STATEMENT 300 TO 1050 THE R MATRIX AND THE VECTOR	CHEM 224
C B ARE CALCUALTED.	CHEM 225
C	CHEM 226
C	CHEM 227
300 YBAR=0.	CHEM 228
IF(JHCODE.EQ.0)GOTO150	CHEM 229
DO 207 I=1,NQ	CHEM 230
AA(I,MM)=ENT1(I)	CHEM 231
207 CONTINUE	CHEM 232
150 DO50I=1,NN	CHEM 233
C	CHEM 234
C	CHEM 235
C YBAR IS THE TOTAL NUMBER OF MOLES OF GAS SPECIES	CHEM 236
C	CHEM 237
C	CHEM 238

50 YBAR=YBAR+Y(I)	CHEM 239
DO10I=1,NN	CHEM 240
FAC=Y(I)/YBAR	CHEM 241
IF(FAC.LT.1.E-73)FAC=1.E-73	CHEM 242
C	CHEM 243
C	CHEM 244
C-----CALCULATE THE FREE ENERGY PARAMETER OF THE GAS SPECIES	CHEM 245
C TO BE MINIMIZE	CHEM 246
C	CHEM 247
C	CHEM 248
FY(I)=Y(I)*(C(I)+ALOG(FAC))	CHEM 249
10 CONTINUE	CHEM 250
IF(KCODE.EQ.0)GOTO111	CHEM 251
C	CHEM 252
C	CHEM 253
C-----IF THERE ARE NO SOLIDS PROCEED TO STATEMENT 111	CHEM 254
C	CHEM 255
C	CHEM 256
C	CHEM 257
C-----CALCULATION OF THE FREE ENERGY PARAMENTER FOR SOLIDS	CHEM 258
C	CHEM 259
C	CHEM 260
DO 11 I=LL,NQ	CHEM 261
FY(I)=Y(I)*FORT(I)	CHEM 262
11 CONTINUE	CHEM 263
C	CHEM 264
C	CHEM 265
C-----PROCEED TO CONSTRUCT THE R MATRIX	CHEM 266
C	CHEM 267
C	CHEM 268
111 DO30J=1,MM1	CHEM 269
DO30K=J,MM1	CHEM 270
SUM=0.	CHEM 271
DO20I=1,NN	CHEM 272

```

20 SUM=SUM+AA(I,J)*AA(I,K)*Y(I)
   R(J,K)=SUM
   R(K,J)=SUM
30 CONTINUE
C
C
C-----GO TO 3000 IF THERE IS NOT AN ENERGY BALANCE CONSTRAINT
C
C
   IF(IHCODE.EQ.0)GOTO3000
   DO 3001 K=1,MM
   SUM=0.
   DO 3002 I=1,NN
3002 SUM=SUM+AA(I,K)*AA(I,MM)*Y(I)
   R(K,MM)=SUM
   R(MM,K)=SUM
3001 CONTINUE
3000 JJ=MM+1
   DO 103 K=1,MM
   SUM=0.
   DO 101 I=1,NN
101 SUM=SUM+AA(I,K)*Y(I)
   R(K,JJ)=SUM
   R(JJ,K)=SUM
103 CONTINUE
   KL=NS-NC+JJ
   DO 1044 J=JJ,KL
   DO 1045 K=JJ,KL
1045 R(J,K)=0.0
1044 CONTINUE
   DO70J=1,MM
C
C
C ----PROCEED TO CALCULATE THE VECTOR B.

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CHEM 305
CHEM 306

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C
C
      SUM=0.
      DO130 I=1,NN
130  SUM=SUM+AA(I,J)*FY(I)
      70 B(J,1)=SUM+BB(J)
      SUM=0.
      DO80 I=1,NN
      80 SUM=SUM+FY(I)
      B(JJ,1)=SUM
      IF(KCODE.EQ.0)GOTO1050
      KK=MM+1
      DO 29 I=LL,NQ
      KK=KK+1
      DO 29 J=1,MM
      R(J,KK)=AA(I,J)
      R(KK,J)=R(J,KK)
      29 CONTINUE
      KM=MM+1
      DO 1053 I=LL,NQ
      KM=KM+1
1053 B(KM,1)=FORT(I)
1050 CONTINUE
      IF(KCODE.EQ.0)R(JJ,JJ)=0.

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C
C
C-----MATRIX INVERSION IS CALLED TO PROVIDE THE SOLUTION FOR
C THE LINEARIZED EQUATIONS. THE SOLUTION OF THE EQUATIONS
C GIVES THE LAGRANGIAN MULTIPLIERS NEEDED TO COMPUTE THE MOLES
C OF EACH GAS SPECIES. THE SOLUTION OF THE EQUATIONS GIVES,
C IN ADDITION, THE MOLES OF EACH SOLID SPECIE.
C
C

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      N=NA

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CHEM 339
CHEM 340

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      M=MA
      CALL MATINV(R,NA,B,MA,NMAX)
      DO100I=1,JJ
C
C      PI(I)=LAGRANGINA MULTIPLIERS
C
      100 PI(I)=B(I,M)
      U=PI(JJ)
      XBAR=U*YBAR
      IF(KCODE.EQ.0)GOTO59
      KK=MM+2
      LW=LL
      DO 1002 J=KK,KL
      X(LW)=B(J,M)
      1002 LW=LW+1
C
C
C-----BETWEEN STATEMENT 59 TO 110 A PROCEDURE IS FOLLOW TO
C      COMPUTE THE NECESSARY DATA TO CALCULATE THE MOLES OF EACH
C      GAS SPECIE.
C
C
      59 DO60I=1,NN
      60 FSUM(I)=-FY(I)+(Y(I)/YBAR)*XBAR
      DO110I=1,NN
      PSUM=0.
      DO120J=1,MM
      120 PSUM=PSUM+PT(J)*AA(I,J)
      YSUM(I)=PSUM*Y(I)
C
C
C-----CALCULATE THE MOLES OF GASEOUS SPECIES
C
C

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CHEM 373
CHEM 374

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110 X(I)=FSUM(I)+YSUM(I)	CHEM 375
C	CHEM 376
C	CHEM 377
C-----COMPUTE THE CONVERGENCE PARAMENTER XLAMBD	CHEM 378
C	CHEM 379
C	CHEM 380
XLAMBD=1.	CHEM 381
DO 86 I=1,NQ	CHEM 382
DELT(I)=X(I)-Y(I)	CHEM 383
IF(DELT(I).GE.0.)GOTO86	CHEM 384
IF(X(I).GT.0.)GOTO86	CHEM 385
XLAM(I)=-Y(I)/DELT(I)	CHEM 386
XLAMBD=AMIN1(XLAMBD,XLAM(I))	CHEM 387
XLAMBD=.99*XLAMBD	CHEM 388
86 CONTINUE	CHEM 389
XLAM1=XLAMBD	CHEM 390
IF(XLAM1.EQ.0.)XLAM1=1.E-5	CHEM 391
DEBAR=0.	CHEM 392
DO87I=1,NN	CHEM 393
87 DEBAR=DEBAR+DELT(I)	CHEM 394
C	CHEM 395
C	CHEM 396
C	CHEM 397
C	CHEM 398
C-----DETERMINE THE SIZE OF THE UNIT VECTOR XLAMBD.	CHEM 399
C APPLY THE CORRECTIONS TO OBTAIN A NEW SET OF ESTIMATES FOR THE	CHEM 400
C NEXT ITERATION. WHEN THE VALUE OF XLAMBD IS VERY SMALL SET THE	CHEM 401
C VALUES OF Y(I) EQUAL TO X(I) TO AVOID USING THE SAME VALUES OF	CHEM 402
C Y(I) AS WAS USED IN THE PREVIOUS ITERATION	CHEM 403
C	CHEM 404
C	CHEM 405
C	CHEM 406
C	CHEM 407
C-----DETERMINE THE FREE ENERGY GRADIENT. IF POSITIVE REDUCE XLAMBD	CHEM 408

```

C
C
93 DFOL=0.
C
C   DFOL=FREE ENERGY GRADIENT
C
      DO88I=1,NQ
      IF(ICODE(I).EQ.1)GOTO83
96  FAC=(Y(I)+XLAMBD*DELT(I))/(YBAR+XLAMBD*DEBAR)
98  IF(FAC.GT.0.)GOTO82
991 XLAMBD=.9*XLAMBD
      IF(XLAMBD.GT.1.0E-09)GOTO96
      IF(FAC.LT.1.E-73)FAC=1.E-73
82  DFOL=DFOL+DELT(I)*(C(I)+ALOG(FAC))
      IF(ICODE(I).EQ.1)GOTO88
      AAA(I)=DELT(I)*(C(I)+ALOG(FAC))
      GOTO88
83  DFOL=DFOL+DELT(I)*FORT(I)
88  CONTINUE
      IF(DFOL.LT.0.000)GOTO89
      XLAMBD=.8*XLAMBD
      IF(XLAMBD.GT.1.0E-08)GOTO93
      DO 881 I=1,NN
881 CONTINUE
C
C
C-----THE VALUE OF XLAMBD THAT ASSURES CONVERGENCE HAS BEEN FOUND
C
C
89  DO76I=1,NQ
      IF(XLAMBD.GT.1.E-6)GOTO90
      IF(DFOL.LT.0.)GOTO90
      IF(XLAM1.LT.1.E-6)XLAM1=1.E-6
C

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CHEM 409
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CHEM 442

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C
C-----CALCULATE THE NEW COMPOSITION FOR THE NEXT ITERATION
C
C      Y(I)=Y(I)+XLAM1*DELT(I)*.1
      GOTO900
90  CONTINUE
      Y(I)=Y(I)+XLAMBDA*DELT(I)
900  CONTINUE
      IF(Y(I).LT.0.)Y(I)=1.E-73
76  CONTINUE
      SUMY=0.
      SUMY1=0.
      DO370 I=1,NN
370  SUMY=SUMY+Y(I)
      IF(KCODE.EQ.0)GOTO372
      DO 371 I=LL,NQ
371  SUMY1=SUMY1+Y(I)
372  SUMY1=SUMY1+SUMY
      DO340 I=1,NQ
      PERC(I)=(Y(I)/SUMY)*100.
      MLFRC(I)=Y(I)/SUMY1
340  PERC1(I)=MLFRC(I)*100.00
C
C
C-----CHECK IF CONVERGENCE CRITERIA HAS BEEN MET. IF NOT GO BACK TO
C      STATEMENT 300.
C
C
C      350 BETA=0.
      GSUM2=0.
      DO 341 I=1,NQ
C      IF(KX.EQ.0.AND.NT.LT.NFREQ)GOTO3410
      IF(Y(I).LT.1.E-30)GOTO534

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CHEM 443
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CHEM 475
CHEM 476

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3410 IF(ICODE(I).EQ.1)GOTO342	CHEM 477
FAC=Y(I)/SUMY	CHEM 478
IF(FAC.LT.1.E-73)FAC=1.E-73	CHEM 479
FY(I)=Y(I)*(C(I)+ALOG(FAC))	CHEM 480
GSUM2=GSUM2+FY(I)	CHEM 481
GOTO341	CHEM 482
342 FY(I)=Y(I)*FORT(I)	CHEM 483
GSUM2=GSUM2+FY(I)	CHEM 484
341 CONTINUE	CHEM 485
IF(XLAMBD.EQ.0.)GOTO534	CHEM 486
3411 DO85I=1,NQ	CHEM 487
85 BETA=BETA+ABS(DELT(I))	CHEM 488
IF(DFDL.GT.0..AND.XLAM1.GE.0.9990)GOTO534	CHEM 489
IF(BETA.LT.XBETA)GOTO800	CHEM 490
532 IF(NTEST.NE.NT)GOTO560	CHEM 491
533 NTEST=NT+NREQ	CHEM 492
534 KCALL=1	CHEM 493
INIT=LL	CHEM 494
NCOUNT=NQ	CHEM 495
C	CHEM 496
C	CHEM 497
C-----PROCEED TO CHECK WHETHER THERE ARE TRACE SPECIES	CHEM 498
C	CHEM 499
C	CHEM 500
CALL HOLD1(KCALL,INIT,NCOUNT,LL)	CHEM 501
560 IF(NT.GE.MAXNT)GOTO600	CHEM 502
NT=NT+1	CHEM 503
C	CHEM 504
C	CHEM 505
C-----IF THE NUMBER OF ITERATIONS EXCEED 900 STOP COMPUTATIONS	CHEM 506
C	CHEM 507
C	CHEM 508
IF(NT.GT.900)GOTO333	CHEM 509
GOTO300	CHEM 510

C	CHEM 511
C	CHEM 512
C-----ADJUST CONVERGENCE CRITERIA. THEY ARE TOO STRINGENT.	CHEM 513
C	CHEM 514
C	CHEM 515
600 XBETA=XBETA+.001	CHEM 516
MAXNT=MAXNT+10	CHEM 517
NT=NT+1	CHEM 518
GOTO300	CHEM 519
800 IF(KOUT.NE.1)GOTO801	CHEM 520
IF(IN.EQ.NC)GOTO801	CHEM 521
C	CHEM 522
C	CHEM 523
C-----COMPUTE THE VALUES OF THE TRACE SPECIES THAT WERE LEFT OUT OF	CHEM 524
C COMPUTATIONS.	CHEM 525
C	CHEM 526
C	CHEM 527
CALL TRACE(PI)	CHEM 528
802 NN=NC	CHEM 529
NQ=NS	CHEM 530
KOUT=0	CHEM 531
KRTRN=0	CHEM 532
C*****	CHEM 533
C*****	CHEM 534
C	* CHEM 535
C	* CHEM 536
C-----CONVERGENCE HAS BEEN ACHIEVED. PRINT OUTPUT	* CHEM 537
C	* CHEM 538
C	* CHEM 539
C*****	CHEM 540
C*****	CHEM 541
801 PRINT 16,NT,U	CHEM 542
16 FORMAT(/1X,30HNT = NO. ITERATIONS REQUIRED = 15.5X,	CHEM 543
1'U=X/Y='1F15.7//)	CHEM 544

DO 2190 J=1,MM	CHEM 545
PRINT 2189,BB(J)	CHEM 546
2189 FORMAT(1X,6HBB(J)=,F15.8)	CHEM 547
2190 CONTINUE	CHEM 548
PRINT201,BETA,SUMY1,H	CHEM 549
201 FORMAT(//1X,7HBETA = E12.4,5X,' TOTAL NO. OF MOLES='F8.4,	CHEM 550
15X,'H='E13.6//)	CHEM 551
PRINT 161,GSUM2	CHEM 552
161 FORMAT(1X,47HFREE ENERGY F(Y) OF THE SYSTEM AT EQUILIBRIUM =E16.8)	CHEM 553
PRINT204,P,T	CHEM 554
204 FORMAT( ///1X, 9HPRESSURE=E13.5,5X,6HTEMP =E13.5//)	CHEM 555
PRINT32	CHEM 556
32 FORMAT(//6X,'I',21X,'Y(I)',9X,'MOLE FRACTION',5X,	CHEM 557
1'MASS FRACTION')	CHEM 558
DO580I=1,NQ	CHEM 559
XMOL(I)=PERC(I)/100.	CHEM 560
580 CONTINUE	CHEM 561
ENTRPY=0.	CHEM 562
XMWGAS=0.	CHEM 563
TMA SMX=0.	CHEM 564
TMASS=0.	CHEM 565
DO81I=1,NQ	CHEM 566
IF(ICODE(I).EQ.1)GOTO790	CHEM 567
TMASS=TMASS+XMW(I)*Y(I)	CHEM 568
XXXX=XMOL(I)*XMW(I)	CHEM 569
XXX=P*XMOL(I)	CHEM 570
S(I)=S(I)-RR*ALOG(XXX)	CHEM 571
ENTRPY=ENTRPY+S(I)*XMOL(I)	CHEM 572
XMWGAS=XMWGAS+XMOL(I)*XMW(I)	CHEM 573
GOTO81	CHEM 574
790 TMA SMX=TMA SMX+XMW(I)*Y(I)	CHEM 575
81 CONTINUE	CHEM 576
TMA SMX=TMA SMX+TMASS	CHEM 577
DO 191I=1,NQ	CHEM 578

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      XMAS1(I)=Y(I)*XMW(I)/TMA SMX
      XMASS(I)=XMW(I)*XMOL(I)/XMWGAS
191  CONTINUE
      DD44I=1,NQ
      IF(IPUNCH.EQ.0)GOTO43
      IF(XMOL(I).LT.1.0000E-4)GOTO43
      PUNCH 46,XMOL(I),SPCIE1(I),SPCIE2(I)
46  FORMAT(2E14.7,10X,2A3)
43  PRINT 19,I,SPCIE1(I),SPCIE2(I),Y(I),XMOL(I),XMASS(I)
44  CONTINUE
19  FORMAT(1X,I6,3X,2A3,2X,3E18.7)
      ENTGAS=0.
      PRINT12
12  FORMAT( ///36X,'MASS FRACTION',/15X,'HEAT OF FORMATION ',2X,
1'OF THE MIXTURE',5X,'ENTROPY')
      DO 781 I=1,NQ
781  ENTGAS=ENTGAS+ENT1(I)*PERC(I)/100.
      DO 79 I=1,NQ
79  PRINT 24, I,SPCIE1(I),SPCIE2(I),ENT(I),XMAS1(I),S(I)
24  FORMAT(1X,I5,3X,2A3,3E17.7)
      ENTRPY=ENTRPY/XMWGAS
      ENTGAS=ENTGAS/XMWGAS
      PRINT18,ENTGAS
18  FORMAT(//1X,'ENTHALPY OF GAS MIXTURE(CAL/GM-MOLE='E17.7)
      PRINT17,XMWGAS,ENTRPY
17  FORMAT(//1X,28HMOLECULAR WEIGHT OF GAS MIX=E16.8,4X,
1'ENTROPY( CAL/(GM-MOLE-OK) )='E17.6//)
      XBETA=CRIT
      LL=NN+1
      NTEST=NFREQ
      KSOLID=0
      KX=0
      IF(IHCODE.EQ.0)GOTO332
      H=H-1000.

```

```

CHEM 579
CHEM 580
CHEM 581
CHEM 582
CHEM 583
CHEM 584
CHEM 585
CHEM 586
CHEM 587
CHEM 588
CHEM 589
CHEM 590
CHEM 591
CHEM 592
CHEM 593
CHEM 594
CHEM 595
CHEM 596
CHEM 597
CHEM 598
CHEM 599
CHEM 600
CHEM 601
CHEM 602
CHEM 603
CHEM 604
CHEM 605
CHEM 606
CHEM 607
CHEM 608
CHEM 609
CHEM 610
CHEM 611
CHEM 612

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      BB(MM)=H/SUMY1
      IF(H.LT.(-30000.))GOTO332
      IF(IHCODE.EQ.1)GOTO500
332   T=T+TINC
      IF(T.GE.3373.)TINC=10.
      IF(T.GE.TMAX)GOTO5
      GOTO500
333   PRINT 5119
5119  FORMAT(1H1)
      STOP
      END

```

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CHEM 613
CHEM 614
CHEM 615
CHEM 616
CHEM 617
CHEM 618
CHEM 619
CHEM 620
CHEM 621
CHEM 622
CHEM 623

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C	SUBROUTINE THERMO	THER	1
C		THER	2
C		THER	3
C	FORMATION OF EVERY CHEMICAL SPECIE AT ANY TEMPERATURE T, AND THE	THER	4
C	SENSIBLE ENTHALPY CHANGE PER MOLE OF EACH SPECIE.	THER	5
C		THER	6
	COMMON/KA/ICODE(40),SPCIE1(40),SPCIE2(40),AA(40,5),	THER	7
	1 ENT1(40),ENT(40)	THER	8
	COMMON/KB/AI(40),BI(40),CI(40),DI(40),EI(40),FI(40),	THER	9
	1 GI(40),AII(40),BII(40),CII(40),DII(40),EII(40),	THER	10
	2 FII(40),GII(40),DELH(40),FORT(40),C(40),TLOW(40),	THER	11
	3 Y(40),XMW(40),MLFRC(40)	THER	12
	COMMON/KBB/CPDT1(5),PERC(40),PERC1(40)	THER	13
	COMMON/KE/S1(5),S2(5),S3(5),S4(5),S5(5),A11(5),A22(5),	THER	14
	1 A33(5),A44(5),A55(5),S6(5),A66(5),JCODE(5),S(40)	THER	15
	COMMON/KF/NC,NS,MM,RR,MM1,NQ,NN,KW,IN,KOUNT,KCODE,KSOLID	THER	16
	COMMON/KG/T,TZERO,TZERO1,TZERO2,TZERO3,TZERO4,TZERO5,P	THER	17
	REAL MLFRC	THER	18
C		THER	19
C	T=TEMPERATURE IN OK	THER	20
C		THER	21
	T1=T	THER	22
	T2=T1*T	THER	23
	T3=T2*T	THER	24
	T4=T3*T	THER	25
	T5=T4*T	THER	26
	A1=T	THER	27
	A2=T2/2.	THER	28
	A3=T3/3.	THER	29
	A4=T4/4.	THER	30
	A5=T5/5.	THER	31
C		THER	32
C		THER	33
		THER	34

C-----	CALCULATE THE FREE ENERGY FUNCTION FORT(I), THE ENTROPY S(I),	THER	35
C	AND THE CHEMICAL ENERGY ENT1(I)	THER	36
C		THER	37
C		THER	38
C		THER	39
C	FORT(I)=FREE ENERGY FUNCTION	THER	40
C	S(I)=ENTROPY	THER	41
C	ENT1(I)=HEAT OF FORMATION AT 298 OK + THE SENSIBLE	THER	42
C	ENTHALPY GAIN FROM 298 TO T.	THER	43
C		THER	44
	NQ=NS	THER	45
	DO 41 I=1,NQ	THER	46
	IF(T.GT.TLOW(I))GOTO6205	THER	47
	FORT(I)=AII(I)*(1.-ALOG(T))-BII(I)*T/2.-CII(I)*T2/6.-DII(I)*T3/12.	THER	48
1	-EII(I)*T4/20.+FII(I)/T-GII(I)	THER	49
	S(I)=(AII(I)*ALOG(T)+BII(I)*T+CII(I)*T2/2.+DII(I)*T3/3.+EII(I)*T4/	THER	50
14.	+GII(I))*RR	THER	51
	ENT1(I)=(AII(I)*A1+BII(I)*A2+CII(I)*A3+DII(I)*A4+EII(I)*A5	THER	52
1	+FII(I))*RR	THER	53
	IF(ICODE(I).EQ.1)GOTO41	THER	54
	C(I)=FORT(I)+ALOG(P)	THER	55
	GOTO41	THER	56
6205	FORT(I)=AI(I)*(1.-ALOG(T))-BI(I)*T/2.-CI(I)*T2/6.-DI(I)*T3/12.	THER	57
1	-EI(I)*T4/20.+FI(I)/T-GI(I)	THER	58
	S(I)=AI(I)*ALOG(T)+BI(I)*T+CI(I)*T2/2.+DI(I)*T3/3.+EI(I)*T4/4.+	THER	59
1	GI(I)	THER	60
	S(I)=S(I)*RR	THER	61
	ENT1(I)=(AI(I)*A1+BI(I)*A2+CI(I)*A3+DI(I)*A4+EI(I)*A5	THER	62
1	+FI(I))*RR	THER	63
	IF(ICODE(I).EQ.1)GOTO41	THER	64
	C(I)=FORT(I)+ALOG(P)	THER	65
41	CONTINUE	THER	66
	DO 78I=1,NQ	THER	67
C	ELEMENTS FOR TEMPERATURES GREATER THAN 1000(OK)	THER	68

IF(I.GT.1)GOTO6291	THER	69
IF(T.LT.TLOW(I))GOTO6207	THER	70
C	THER	71
C	THER	72
C-----CALCULATE THE SENSIBLE ENTHALPY OF THE CONSTITUENT	THER	73
C	THER	74
C	THER	75
DO 296J=1,MM1	THER	76
CPDT1(J)=(S1(J)*A1+S2(J)*A2+S3(J)*A3+S4(J)*A4+S5(J)*A5	THER	77
1 +S6(J))*RR	THER	78
296 CONTINUE	THER	79
GOTO6291	THER	80
C	THER	81
C	THER	82
C-----CALCULATE THE SENSIBLE ENTHALPY OF THE CONSTITUENT	THER	83
C ELEMENTS FOR TEMPERATURES LESS THAN 1000(OK).	THER	84
C	THER	85
C	THER	86
6207 DO297J=1,MM1	THER	87
CPDT1(J)=(A11(J)*A1+A22(J)*A2+A33(J)*A3+A44(J)*A4	THER	88
1 +A55(J)*A5+A66(J))*RR	THER	89
297 CONTINUE	THER	90
C	THER	91
C RSUM IS THE SENSIBLE ENTHALPY OF THE ELEMENTS OF THE ITH SPECIE	THER	92
C AT TEMPERATURE T(OK),WITH RESPECT TO THE STANDARD STATE(P=1ATM,	THER	93
C TZERO=298.15OK)	THER	94
C	THER	95
C	THER	96
C-----COMPUTE THE HEAT OF FORMATION OF EACH CHEMICAL SPECIE	THER	97
C	THER	98
C	THER	99
C	THER	100
C ENT(I)=HEAT OF FORMATION OF EACH CHEMICAL SPECIE AT TEMPERATURE	THER	101
C T.	THER	102



C

```
6291 RSUM=0.  
    DO 398 J=1,MM1  
      IF(JCODE(J).EQ.1)GOTO393  
      RSUM=RSUM+0.5*AA(I,J)*CPDT1(J)  
    GO TO 398  
393 RSUM=RSUM+AA(I,J)*CPDT1(J)  
398 CONTINUE  
    ENT(I)=ENT1(I)-RSUM  
    IF(ABS(ENT(I)).LT.3.)ENT(I)=0.  
78 CONTINUE  
    RETURN  
    END
```

```
THER 103  
THER 104  
THER 105  
THER 106  
THER 107  
THER 108  
THER 109  
THER 110  
THER 111  
THER 112  
THER 113  
THER 114  
THER 115
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XBI(J)=BI(K)
XBII(J)=BII(K)
XCI(J)=CI(K)
XCII(J)=CII(K)
XDI(J)=DI(K)
XDII(J)=DII(K)
XEI(J)=EI(K)
XEII(J)=EII(K)
XFI(J)=FI(K)
XFII(J)=FII(K)
XGI(J)=GI(K)
XGII(J)=GII(K)
XC(J)=C(K)
XPERC(J)=PERC(K)
XPERC1(J)=PERC1(K)
XMLFR(J)=MLFRC(K)
XFORT(J)=FORT(K)
XENT(J)=ENT(K)
XENT1(J)=ENT1(K)
XTLOW(J)=TLOW(K)
XDELH(J)=DELH(K)
XXMW(J)=XMW(K)
XPCIE1(J)=SPCIE1(K)
XPCIE2(J)=SPCIE2(K)
IICODE(J)=ICODE(K)
DO540I=1,MM
540 XAA(J,I)=AA(K,I)
530 CONTINUE
LI=NN
521 DO 510 I=1,LI
    AI(I)=XAI(I)
    AII(I)=XAII(I)
    BI(I)=XBI(I)
    BII(I)=XBII(I)

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HOLD 35
HOLD 36
HOLD 37
HOLD 38
HOLD 39
HOLD 40
HOLD 41
HOLD 42
HOLD 43
HOLD 44
HOLD 45
HOLD 46
HOLD 47
HOLD 48
HOLD 49
HOLD 50
HOLD 51
HOLD 52
HOLD 53
HOLD 54
HOLD 55
HOLD 56
HOLD 57
HOLD 58
HOLD 59
HOLD 60
HOLD 61
HOLD 62
HOLD 63
HOLD 64
HOLD 65
HOLD 66
HOLD 67
HOLD 68

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      CI(I)=XCI(I)
      CII(I)=XCII(I)
      DI(I)=XDI(I)
      DII(I)=XDII(I)
      EI(I)=XEI(I)
      EII(I)=XEII(I)
      FI(I)=XFI(I)
      FII(I)=XFII(I)
      GI(I)=XGI(I)
      GII(I)=XGII(I)
      SPCIE1(I)=XPCIE1(I)
      SPCIE2(I)=XPCIE2(I)
      FORT(I)=XFORT(I)
      ENT(I)=XENT(I)
      ENT1(I)=XENT1(I)
      TLOW(I)=XTLOW(I)
      DELH(I)=XDELH(I)
      XMW(I)=XXMW(I)
      ICODE(I)=IICODE(I)
      PERC(I)=XPERC(I)
      PERC1(I)=XPERC1(I)
      MLFR(I)=XMLFR(I)
      IF(ICODE(I).EQ.1)GOTO5211
      C(I)=XC(I)
5211 DO 590 J=1,MM
      590 AA(I,J)=XAA(I,J)
      KOUT=1
      510 Y(I)=XY(I)
      KW=0
      IN=NN
      DO550I=1,NN
      IF(PERC(I).GT.1.E-9)GOTO550
5500 IN=IN-1
      KW=KW+1

```

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HOLD 69
HOLD 70
HOLD 71
HOLD 72
HOLD 73
HOLD 74
HOLD 75
HOLD 76
HOLD 77
HOLD 78
HOLD 79
HOLD 80
HOLD 81
HOLD 82
HOLD 83
HOLD 84
HOLD 85
HOLD 86
HOLD 87
HOLD 88
HOLD 89
HOLD 90
HOLD 91
HOLD 92
HOLD 93
HOLD 94
HOLD 95
HOLD 96
HOLD 97
HOLD 98
HOLD 99
HOLD 100
HOLD 101
HOLD 102

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550 CONTINUE
    NN=IN
    NL=NN+1
    IF(KCODE.EQ.0)GOTO5600
5050 DO 507 I=INIT,NCOUNT
    IF(KCALL.EQ.2)GOTO5051
    AI(NL)=AI(I)
    AII(NL)=AII(I)
    BI(NL)=BI(I)
    BII(NL)=BII(I)
    CI(NL)=CI(I)
    CII(NL)=CII(I)
    DI(NL)=DI(I)
    DII(NL)=DII(I)
    EI(NL)=EI(I)
    EII(NL)=EII(I)
    FI(NL)=FI(I)
    FII(NL)=FII(I)
    GI(NL)=GI(I)
    GII(NL)=GII(I)
    SPCIE1(NL)=SPCIE1(I)
    SPCIE2(NL)=SPCIE2(I)
    FORT(NL)=FORT(I)
    ICODE(NL)=ICODE(I)
    XMW(NL)=XMW(I)
    ENT(NL)=ENT(I)
    ENT1(NL)=ENT1(I)
    TLOW(NL)=TLOW(I)
    DELH(NL)=DELH(I)
    PERC(NL)=PERC(I)
    PERC1(NL)=PERC1(I)
    MLFRC(NL)=MLFRC(I)
    IF(KSOLID.EQ.1)GOTO551
5051 XAI(I)=AI(I)

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HOLD 103
HOLD 104
HOLD 105
HOLD 106
HOLD 107
HOLD 108
HOLD 109
HOLD 110
HOLD 111
HOLD 112
HOLD 113
HOLD 114
HOLD 115
HOLD 116
HOLD 117
HOLD 118
HOLD 119
HOLD 120
HOLD 121
HOLD 122
HOLD 123
HOLD 124
HOLD 125
HOLD 126
HOLD 127
HOLD 128
HOLD 129
HOLD 130
HOLD 131
HOLD 132
HOLD 133
HOLD 134
HOLD 135
HOLD 136

```

XAII(I)=AII(I)	HOLD 137
XBII(I)=BII(I)	HOLD 138
XCII(I)=CII(I)	HOLD 139
XCI(I)=CI(I)	HOLD 140
XCII(I)=CII(I)	HOLD 141
XDI(I)=DI(I)	HOLD 142
XDII(I)=DII(I)	HOLD 143
XEI(I)=EI(I)	HOLD 144
XEII(I)=EII(I)	HOLD 145
XFI(I)=FI(I)	HOLD 146
XFII(I)=FII(I)	HOLD 147
XGI(I)=GI(I)	HOLD 148
XGII(I)=GII(I)	HOLD 149
XPCIE1(I)=SPCIE1(I)	HOLD 150
XPCIE2(I)=SPCIE2(I)	HOLD 151
XPERC(I)=PERC(I)	HOLD 152
XPERC1(I)=PERC1(I)	HOLD 153
XMLFR(I)=MLFRC(I)	HOLD 154
XFORT(I)=FORT(I)	HOLD 155
IICODE(I)=ICODE(I)	HOLD 156
XXMW(I)=XMW(I)	HOLD 157
XTLOW(I)=TLOW(I)	HOLD 158
XDELH(I)=DELH(I)	HOLD 159
IF(KCALL.EQ.2)GOTO551	HOLD 160
XENT(I)=ENT(I)	HOLD 161
XENT1(I)=ENT1(I)	HOLD 162
551 DO 591 J=1,MM	HOLD 163
IF(KCALL.EQ.2)GOTO5510	HOLD 164
AA(NL,J)=AA(I,J)	HOLD 165
IF(KSOLID.EQ.1)GOTO591	HOLD 166
5510 XAA(I,J)=AA(I,J)	HOLD 167
591 CONTINUE	HOLD 168
IF(KCALL.EQ.2)GOTO560	HOLD 169
Y(NL)=Y(I)	HOLD 170

```
      NL=NL+1
507  CONTINUE
      KSOLID=1
5600 LL=NN+1
      NQ=NQ-KW
      IF(KCODE.EQ.0)NQ=NN
560  RETURN
      END
```

```
HOLD 171
HOLD 172
HOLD 173
HOLD 174
HOLD 175
HOLD 176
HOLD 177
HOLD 178
```

SUBROUTINE TRACE (PI)	TRAC	1
COMMON/KA/ICODE(40),SPCIE1(40),SPCIE2(40),AA(40,5),	TRAC	2
1 ENT1(40),ENT(40)	TRAC	3
COMMON/K8/AI(40),BI(40),CI(40),DI(40),EI(40),FI(40),	TRAC	4
1 GI(40),AII(40),BII(40),CII(40),DII(40),EII(40),	TRAC	5
2 FII(40),GII(40),DELH(40),FORT(40),C(40),TLOW(40),	TRAC	6
3 Y(40),XMW(40),MLFRC(40)	TRAC	7
COMMON/KBB/CPDT1(5),PERC(40),PERC1(40)	TRAC	8
COMMON/KC/IICODE(40),XPCIE1(40),XPCIE2(40),XAA(40,5),	TRAC	9
1 XENT(40),XENT1(40)	TRAC	10
COMMON/KD/XAI(40),XBI(40),XCI(40),XDI(40),XEI(40),	TRAC	11
1 XFI(40),XGI(40),XAI1(40),XBI1(40),XCI1(40),	TRAC	12
2 XDII(40),XEII(40),XFII(40),XGII(40),XMLFR(40)	TRAC	13
COMMON/KDD/XDELH(40),XCPDT(40),XCPDT1(05),XFORT(40),	TRAC	14
1XY(40),XC(40),XTLOW(40),XXMW(40),XPERC(40),XPERC1(40)	TRAC	15
COMMON/KF/NC,NS,MM,RR,MM1,NQ,NN,KW,IN,KOUT,KCODE,KSOLID	TRAC	16
DIMENSION YTRACE(40),PI(7)	TRAC	17
REAL MLFRC	TRAC	18
L1=IN+1	TRAC	19
C	TRAC	20
C STORE THE VALUES OF Y(I) OF THE SOLID SPECIES BEFORE BEING ERASED	TRAC	21
C BY THE CALCULATIONS OF THE TRACE SPECIES WHICH FOLLOWS.	TRAC	22
C	TRAC	23
IF(KCODE.EQ.0)GOTO7428	TRAC	24
NP=NC+1	TRAC	25
L4=NN+1	TRAC	26
DO 7427 I=L4,NQ	TRAC	27
XY(NP)=Y(I)	TRAC	28
XPERC(NP)=PERC(I)	TRAC	29
XMLFR(NP)=MLFRC(I)	TRAC	30
XPERC1(NP)=PERC1(I)	TRAC	31
7427 NP=NP+1	TRAC	32
7428 YBAR=0.	TRAC	33
C	TRAC	34



C        PROCEED TO CALCULATE THE TRACE SPECIES.

C

C

```
      DO 7429 I=1,NN
7429  YBAR=YBAR+Y(I)
      DO 7433 I=L1,NC
      SUM=0.
      DO 7430 J=1,MM1
7430  SUM=SUM+XAA(I,J)*PI(J)
      SUM1=-C(I)+SUM
      IF(SUM1.LT.0.)GOTO7431
      YTRACE(I)=YBAR*(EXP(SUM1))
      GOTO7432
7431  SUM2=-SUM1
      YTRACE(I)=YBAR*(1./(EXP(SUM2)))
      XPERC(I)=(YTRACE(I)/YBAR)*100.
7432  XY(I)=YTRACE(I)
7433  CONTINUE
      DO 7434 I=1,NN
      XPERC(I)=PERC(I)
7434  XY(I)=Y(I)
      L1=NS
521  DO 510 I=1,L1
      AI(I)=XAI(I)
      AII(I)=XAII(I)
      BI(I)=XBI(I)
      BII(I)=XBII(I)
      CI(I)=XCI(I)
      CII(I)=XCII(I)
      DI(I)=XDI(I)
      DII(I)=XDII(I)
      EI(I)=XEI(I)
      EII(I)=XEII(I)
      FI(I)=XFI(I)
```

TRAC	35
TRAC	36
TRAC	37
TRAC	38
TRAC	39
TRAC	40
TRAC	41
TRAC	42
TRAC	43
TRAC	44
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TRAC	46
TRAC	47
TRAC	48
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TRAC	50
TRAC	51
TRAC	52
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TRAC	56
TRAC	57
TRAC	58
TRAC	59
TRAC	60
TRAC	61
TRAC	62
TRAC	63
TRAC	64
TRAC	65
TRAC	66
TRAC	67
TRAC	68

```

      FII(I)=XFII(I)
      GI(I)=XGI(I)
      GII(I)=XGII(I)
      SPCIE1(I)=XPCIE1(I)
      SPCIE2(I)=XPCIE2(I)
      FORT(I)=XFORT(I)
      ENT(I)=XENT(I)
      ENT1(I)=XENT1(I)
      TLOW(I)=XTLOW(I)
      DELH(I)=XDELH(I)
      XMW(I)=XXMW(I)
      ICODE(I)=IICODE(I)
      PERC(I)=XPERC(I)
      PERC1(I)=XPERC1(I)
      MLFRC(I)=XMLFR(I)
      IF(ICODE(I).EQ.1)GOTO5211
      C(I)=XC(I)
5211 DO 590 J=1,MM
      590 AA(I,J)=XAA(I,J)
      510 Y(I)=XY(I)
      RETURN
      END

```

```

TRAC 69
TRAC 70
TRAC 71
TRAC 72
TRAC 73
TRAC 74
TRAC 75
TRAC 76
TRAC 77
TRAC 78
TRAC 79
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TRAC 82
TRAC 83
TRAC 84
TRAC 85
TRAC 86
TRAC 87
TRAC 88
TRAC 89
TRAC 90

```

C	SUBROUTINE MATINV(A,N,B,M,NMAX)	MATI	1
C		MATI	2
C		MATI	3
C	MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF LINEAR EQUATIONS	MATI	4
	DIMENSION A(7,7),B(7,1),IPIVOT(7),INDEX(7,2)	MATI	5
	EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUM), (AMAX,T,SWAP)	MATI	6
C		MATI	7
C	INITIALIZATION	MATI	8
C		MATI	9
	5 ISCALE=0	MATI	10
	6 R1=10.0**18	MATI	11
	7 R2=1.0/R1	MATI	12
	10 DETERM=1.0	MATI	13
	15 DO 20 J=1,N	MATI	14
	20 IPIVOT(J)=0	MATI	15
	30 DO 550 I=1,N	MATI	16
C		MATI	17
C	SEARCH FOR PIVOT ELEMENT	MATI	18
C		MATI	19
	40 AMAX=0.0	MATI	20
	45 DO 105 J=1,N	MATI	21
	50 IF (IPIVOT(J)-1)60,105,60	MATI	22
	60 DO 100 K=1,N	MATI	23
	70 IF (IPIVOT(K)-1)80,100,740	MATI	24
	80 IF (ABS(AMAX)-ABS(A(J,K)))85,100,100	MATI	25
	85 IROW=J	MATI	26
	90 ICOLUM=K	MATI	27
	95 AMAX=A(J,K)	MATI	28
	100 CONTINUE	MATI	29
	105 CONTINUE	MATI	30
	IF (AMAX)110,106,110	MATI	31
	106 DETERM=0.0	MATI	32
	ISCALE=0	MATI	33
	GO TO 740	MATI	34

110	IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1	MATI	35
C		MATI	36
C	INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL	MATI	37
C		MATI	38
130	IF (IROW-ICOLUM)140,260,140	MATI	39
140	DETERM=-DETERM	MATI	40
150	DO 200 L=1,N	MATI	41
160	SWAP=A(IROW,L)	MATI	42
170	A(IROW,L)=A(ICOLUM,L)	MATI	43
200	A(ICOLUM,L)=SWAP	MATI	44
205	IF(M)260,260,210	MATI	45
210	DO 250 L=1,M	MATI	46
220	SWAP=B(IROW,L)	MATI	47
230	B(IROW,L)=B(ICOLUM,L)	MATI	48
250	B(ICOLUM,L)=SWAP	MATI	49
260	INDEX(I,1)=IROW	MATI	50
270	INDEX(I,2)=ICOLUM	MATI	51
310	PIVOT=A(ICOLUM,ICOLUM)	MATI	52
C		MATI	53
C	SCALE THE DETERMINANT	MATI	54
C		MATI	55
1000	PIVOTI=PIVOT	MATI	56
1005	IF(ABS(DETERM)-R1)1030,1010,1010	MATI	57
1010	DETERM=DETERM/R1	MATI	58
	ISCALE=ISCALE+1	MATI	59
	IF(ABS(DETERM)-R1)1060,1020,1020	MATI	60
1020	DETERM=DETERM/R1	MATI	61
	ISCALE=ISCALE+1	MATI	62
	GO TO 1060	MATI	63
1030	IF(ABS(DETERM)-R2)1040,1040,1060	MATI	64
1040	DETERM=DETERM*R1	MATI	65
	ISCALE=ISCALE-1	MATI	66
	IF(ABS(DETERM)-R2)1050,1050,1060	MATI	67
1050	DETERM=DETERM*R1	MATI	68

```

        ISCALE=ISCALE-1
1060 IF(ABS(PIVOTI)-R1)1090,1070,1070
1070 PIVOTI=PIVOTI/R1
        ISCALE=ISCALE+1
        IF(ABS(PIVOTI)-R1)320,1080,1080
1080 PIVOTI=PIVOTI/R1
        ISCALE=ISCALE+1
        GO TO 320
1090 IF(ABS(PIVOTI)-R2)2000,2000,320
2000 PIVOTI=PIVOTI*R1
        ISCALE=ISCALE-1
        IF(ABS(PIVOTI)-R2)2010,2010,320
2010 PIVOTI=PIVOTI*R1
        ISCALE=ISCALE-1
320 DETERM=DETERM*PIVOTI
C
C      DIVIDE PIVOT ROW BY PIVOT ELEMENT
C
330 A(ICOLUM,ICOLUM)=1.0
340 DO 350 L=1,N
350 A(ICOLUM,L)=A(ICOLUM,L)/PIVOT
355 IF(M) 380,380,360
360 DO 370 L=1,M
370 B(ICOLUM,L)=B(ICOLUM,L)/PIVOT
C
C      REDUCE NON-PIVOT ROWS
C
380 DO 550 L1=1,N
390 IF(L1-ICOLUM)400,550,400
400 T=A(L1,ICOLUM)
420 A(L1,ICOLUM)=0.0
430 DO 450 L=1,N
450 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T
455 IF(M) 550,550,460

```

```

MATI 69
MATI 70
MATI 71
MATI 72
MATI 73
MATI 74
MATI 75
MATI 76
MATI 77
MATI 78
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MATI 87
MATI 88
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MATI 90
MATI 91
MATI 92
MATI 93
MATI 94
MATI 95
MATI 96
MATI 97
MATI 98
MATI 99
MATI 100
MATI 101
MATI 102

```

```

460 DO 500 L=1,M
500 B(L1,L)=B(L1,L)-B(JCOLUM,L)*T
550 CONTINUE
C
C   INTERCHANGE COLUMNS
600 DO 710 I=1,N
C
610 L=N+1-I
620 IF (INDEX(L,1)-INDEX(L,2))630,710,630
630 JROW=INDEX(L,1)
640 JCOLUM=INDEX(L,2)
650 DO 705 K=1,N
660 SWAP=A(K,JROW)
670 A(K,JROW)=A(K,JCOLUM)
700 A(K,JCOLUM)=SWAP
705 CONTINUE
710 CONTINUE
740 RETURN
END

```

```

MATI 103
MATI 104
MATI 105
MATI 106
MATI 107
MATI 108
MATI 109
MATI 110
MATI 111
MATI 112
MATI 113
MATI 114
MATI 115
MATI 116
MATI 117
MATI 118
MATI 119
MATI 120
MATI 121

```

# CHEMICAL EQUILIBRIUM ANALYSIS NOMENCLATURE

## MAIN:

AA(I,J): Formula number. Gives the gram atoms of element J in Species I.

AI...GI: These are the seven empirical constants for the high temperature fit ( $1000^{\circ}\text{K}$ - $6000^{\circ}\text{K}$ ) for the free energy functions. The first five constants (AI through EI) are used for the heat capacity fit.

AII...GII: These are the seven empirical constants for the low temperature fit ( $300^{\circ}\text{K}$ - $1000^{\circ}\text{K}$ ) for the free energy function.

All...A66: These are the six empirical constants for the Enthalpy fit of the constituent elements ( $300^{\circ}\text{K}$ - $1000^{\circ}\text{K}$ ).

B(J,1): Is the vector formed from the right hand side of Equations in Table 4-1.

BB(J): Gram atoms of the constituent element J.

BETA: Criteria for convergence. It varies if convergence has not been achieved after 100 iterations.

C(I): Defined by Equation (4-12).

CRIT: Initial criteria for convergence.

DELT(I): Difference between the values of Y(I) and the calculated value of X(I) (gram/moles).

DFDL: Is the gradient  $dF/d\lambda$  defined by Equation (4-41).

DEBAR: Is the sum of DELT(I) (gram/moles).

ENT(I): Is the heat of formation of species I, (calories/gram-mole).

ENTL(I): The enthalpy of each species I, (calories/gram-mole).

ENTGAS: The total enthalpy of the gas mixture, (calories/gram-mole).

ENTRPY: The total entropy of the gas mixture, (calories/gram-mole  $^{\circ}\text{K}$ ).

FY(I): Defined by Equation (4-11).

FORT(I): Is  $\bar{F}_T^0/RT$ .

FSUM(I): Is the sum of the first two terms of the right hand side of Equation (4-32).

GSUM2: Is the total free energy of the system at equilibrium, (calories/gram-mole).

H: This variable is used for restricted equilibrium, and is the heat balance constraint (cal/gram-mole of polymer).

ICODE(I): Is a code used to identify whether a specie is a gas or a solid. If ICODE is zero, the species is a gas. If ICODE is one, the species is a solid.

IPUNCH: If IPUNCH is one, punch output. Otherwise, IPUNCH is zero.

JCODE: Is a code used to identify whether the reference state of the constituent elements are in the gas or in the solid state.

KOUT: When KOUT is zero, trace species computations are bypassed. When KOUT is one, trace species are computed after convergence to equilibrium has been achieved.

KCODE: When the system is an all gas system KCODE is



is zero. When there is a solid, KCODE is one. This is used to adjust the size of the matrix that needs to be inverted.

MM: Is the number of elements.

MAXNT: Number of iterations after which the criteria for convergence CRIT is adjusted.

MLFRC(I): Mole fraction of species I in the mixture.

NA: Is the size of the R matrix.

NC: Number of gas species read in.

NN: Number of gas species remaining after trace species are eliminated.

NQ: Is the total number of gas and solid species after trace species are eliminated.

NS: Is the total number of gas and solid species read in.

NT: Total number of iterations.

NFREQ: Number of iterations after which the system is checked for trace species.

P: Pressure of the system in atmosphere.

PI: The Lagrange Multipliers.

R: Is the matrix formed from the coefficients of the Equations in Table 4-1.

S(I): Entropy of species I.

S1...S6: These are the six empirical constants for the enthalpy fit of the constituent elements (1000°K-6000°K).

SPECIE(I): Specie identification number.

T: Temperature in  $^{\circ}\text{K}$ .

TLOW(I): Maximum temperature of low temperature fit for species I.

X(I): Calculated value of the moles of species I.

XMW(I): Molecular weight of species I.

Y(I): Moles of Y(I) guessed; or improved values of Y(I), based on the calculated values of X(I).

THERMO: Only those variables not previously defined will be mentioned in this section. This subroutine calculates the thermodynamic properties of the gas-solid system.

ENT1(I): Enthalpy of species I. (Calories/gram-mole).

CPDT1(J): Sensible enthalpy gain by the constituent elements. (Calories/gram-mole).

HOLD1: This subroutine stores the variables of the trace species in temporary location.

IICODE(I): Temporary location of ICODE(I).

XAA(I,J): Temporary storage for AA(I,J).

XAI...XGI: Temporary storage location for AI...GI.

XC(I): Temporary storage location for C(I).

XXMW(I): Temporary storage location for XMW(I).

XFORT(I): Temporary location for FORT(I).

XPCIE1(I): Temporary storage location for SPCIE1(I).

TRACE: This subroutine computes the value of the trace species once convergence to the minimum free energy has been achieved.

YTRACE(I): Value of the moles of Y(I) calculated for

the trace species.

# INPUT FORMAT FOR THE CHEMICAL EQUILIBRIUM PROGRAM

This program calculates the equilibrium composition of any system at specified temperatures and pressures. Multiple cases can be run with the same data base by specifying the initial temperature at which equilibrium composition is desired, the temperature increment and the final temperature.

CARD 1:      FORMAT (5F10.4,3I6)                      COLUMNS:

XT = Initial Temperature ( $^{\circ}\text{K}$ ).                      1-10

TMAX = Final Temperature ( $^{\circ}\text{K}$ ).                      11-20

TINC = Temperature Increment ( $^{\circ}\text{K}$ )                      21-30

CRIT = Convergence Tolerance (0.001  
   moles is recommended).                      31-40

TZERO = Reference Temperature (298.16 $^{\circ}\text{K}$ )                      41-50

NC = Number of Gas Components                      51-56

MM = Number of Elements                      57-62

NNS = Number of Solid Species                      63-68

CARD 2:      FORMAT (I6, F10.5, I3)

IHCODE = 1 (Restrictive Equilibrium Option)  
   otherwise, leave blank.                      6

H = Enthalpy for Restrictive Equilibrium Option.                      7-16

IPUNCH = 1, Punch Mole Fraction and  
   species name, otherwise,  
   leave blank.                      19

CARD 3:      Reads the empirical constants for the heat capacity of the reference elements for the temperature range

1000<sup>o</sup>K to 6000<sup>o</sup>K. These are stored in the constants S1 through S6. If the reference element is a solid, JCODE should be set to one. CARD 3 is read MM number of times.

CARD 3:    FORMAT (6E10.4, I3)                      COLUMNS:

S1(J) =	Empirical constants for the heat capacity of the refe- rence elements for the temperature range 1000 <sup>o</sup> K to 6000 <sup>o</sup> K.	1-10
S2(J) =		11-20
S3(J) =		11-20
S4(J) =		21-30
S5(J) =		31-40
S6(J) =		51-60

JCODE(J) = Zero if reference element is  
                  a gas, one if it is a solid  
                  or a liquid.

66

CARD 4:    FORMAT (6E10.4)

A11(J) =	Empirical constants for the heat capacity of the refe- rence elements for the temperature range 298 <sup>o</sup> K to 1000 <sup>o</sup> K.	1-10
A22(J) =		11-20
A33(J) =		21-30
A44(J) =		31-40
A55(J) =		41-50
A66(J) =		51-60

CARD 4, as with CARD 3, is read in MM number of times.

CARD 5:    FORMAT (10x, 3E10.4, 2x, 2A3, I4)

TLOW(I) = Maximum temperature of low tem-	
perature fit (usually 1000 <sup>o</sup> K)	11-20
YMW(I) = Molecular weight of species	21-30

COLUMNS:

Y(I) = Mole fraction of species	31-40
SPCIE1(I) = Alphameric representation	
SPCIE2(I) = of chemical species	41-43
ICODE(I) = Zero for a gas, one for a solid or liquid species.	51

CARD 6:   FORMAT (7E10.4)

AI(I) =		1-10
BI(I) =	Empirical constants for the free energy fit of the che- mical species for the temperature range of 1000 <sup>o</sup> K to 6000 <sup>o</sup> K.	11-20
CI(I) =		21-30
DI(I) =		31-40
EI(I) =		41-50
FI(I) =		51-60
GI(I) =		61-70

CARD 7:   FORMAT (7E10.4)

AII(I) =		1-10
BII(I) =	Empirical constants for the free energy fit of the che- mical species for the temperature range of 298 <sup>o</sup> K to 1000 <sup>o</sup> K.	11-20
CII(I) =		21-30
DII(I) =		31-40
EII(I) =		41-50
FII(I) =		51-60
GII(I) =		61-70

CARD 8:   FORMAT (8E10.4)

AA(I,1) =		1-10
AA(I,2) =	Formula number of the Ith species (continued).	11-20

COLUMNS:

AA(I,3) =	Formula number for the	21-30
AA(I,4) =	Ith species.	31-40
AA(I,M) =		71-80

CARDS 5, 6, 7 and 8 are read.

CARD 9:   FORMAT (2F14.8)

RR = 1.98726	1-14
--------------	------

P = Pressure in atmospheres.	15-28
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CARD 10:   FORMAT (I6)

NFREQ = Maximum number of iterations.	1-6
---------------------------------------	-----

TABLE E-2. Typical Chemical Equilibrium Input Data

10	2	4	1	2	5500.	DATA	1
2160.			500.		.8 0.3500000 .00000100	DATA	2
.50000E9			.50000E5		.4805555E-12 0.90	DATA	3
3000.0E0	1073.00		2.E-4			DATA	4
1.363252E01	1.85605E-3	-7.6675E-7	1.151043E-9	-1.139E-14	-6.49672E2	DATA	5
-7.12442E07	3.34065E-3	-5.5262E-6	1.51400E-9	-2.382E-14	-6.80533E1	DATA	6
3.043690E06	1.1871E-4	-7.3994E-9	-2.033E-11	2.4594E-15	-8.54910E2	DATA	7
2.846085E04	1.9321E-3	-9.6119E-6	9.51227E-9	-3.309E-12	-9.67253E2	DATA	8
3.597613E07	8.1456E-4	-2.2387E-7	4.2490E-11	-3.346E-15	-1.19279E3	DATA	9
3.718995E0	-2.5167E-3	8.58374E-6	-8.2999E-9	2.7082E-12	-1.10577E3	DATA	10
2.220792E01	1.74309E-3	-1.2008E-6	5.0841E-10	-8.169E-14	-7.49661E2	DATA	11
4.245929E01	1.1866E-2	-1.9539E-5	1.6109E-08	-4.991E-12	-4.80666E2	DATA	12
1000.00E0	15.0350E0	.30420E-4	CH3	0		DATA	13
2.802766E06	2.5045E-3	-2.2892E-6	3.8993E-10	-2.528E-14	1.578749E45.684117E0	DATA	14
3.399505E04	2.6783E-3	2.03327E-7	-1.155E-09	4.1288E-13	1.564979E42.703747E0	DATA	15
1.00000E0	3.00000E0					DATA	16
1000.00E0	1.6043E01	.38328E-3	CH4	0		DATA	17
1.18000E0	1.0950E-2	-4.0620E-6	7.137E-10	-4.749E-14	-9.85556E03 1.2506E01	DATA	18
4.249768E0	-6.9127E-3	3.1602E-5	-2.9715E-8	9.5103E-12	-1.01866E4-9.1755E-1	DATA	19
1.00000E0	4.00000E0					DATA	20
1000.00E0	2.6038E01	.17288E-2	C2H2	0		DATA	21
4.4966E00	5.2698E-3	-1.840E-06	3.1054E-10	-2.000E-14	2.5637E004-3.14481E0	DATA	22
7.90333E-1	2.3466E-2	-3.5542E-5	2.7951E-8	-8.448E-12	2.6255E04 1.4005E01	DATA	23
2.00000E0	2.00000E0					DATA	24
1000.00E0	2.01600E0	2.00385E0	H2	0		DATA	25
3.04369E00	6.1187E-4	-7.399E-9	-2.03E-11	2.459E-15	-8.5491E02 -1.648E00	DATA	26
2.846085E04	1.932E-03	-9.6119E-6	9.5123E-09	-3.309E-12	-9.67254E2 -1.4118E0	DATA	27
0.E0	2.E0					DATA	28
1000.00E0	1.00800E0	.47481E-2	H	0		DATA	29
2.500000E0	0.00000E0	0.00000E0	0.00000E0	0.00000E0	2.547050E4-4.6001E-1	DATA	30
2.500000E0	0.00000E0	0.00000E0	0.00000E0	0.00000E0	2.547050E4-4.6001E-1	DATA	31
0.E0	1.E0					DATA	32
1000.00E0	18.0160E0	.10954E-3	H2O	0		DATA	33
						DATA	34



2.67075E0	3.0317E-3	-8.535E-7	1.179E-10	-6.197E-15	-2.9889E04	6.88383E0	DATA	35
4.15650E00	-1.7244E-35	6.982E-06	-4.5930E-91	4.234E-12	-3.02888E4	-6.8616E-1	DATA	36
0.E0	2.0E0	1.E0					DATA	37
1000.00E0	2.8011E01	1.97510E0	CO	0			DATA	38
2.9512E00	1.5526E-3	-6.1911E-7	1.135E-10	-7.788E-15	-1.4232E04	6.5314E00	DATA	39
3.787133E0	-2.171E-035	0.7573E-6	-3.4738E-97	7.217E-13	-1.43635E4	2.63355E0	DATA	40
1.E0	0.E0	1.0E0					DATA	41
1000.00E0	44.011E0	.23651E-4	CO2	0			DATA	42
4.4129E003	1.923E-03	-1.298E-6	2.415E-10	-1.674E-14	-4.8944E04	-7.2876E-1	DATA	43
2.170100E0	1.0378E-2	-1.0734E-56	3.4592E-9	-1.628E-12	-4.83526E4	1.06644E1	DATA	44
1.E0	0.E0	2.0E0					DATA	45
1000.00E0	29.09800	.17321E-3	SIH	0			DATA	46
3.067823E01	1.50816E-3	-5.8923E-7	1.08543E-9	-7.476E-15	4.402100E45	9.16108E0	DATA	47
4.236578E0	-4.3652E-39	6.9889E-6	-7.5517E-92	0.0693E-12	4.385927E46	0.06156E-1	DATA	48
0.0E0	1.E0	0.E0	1.E0				DATA	49
1000.00E0	44.0900E0	.306063E0	SIO	0			DATA	50
3.729516E08	6.3359E-4	-3.5894E-76	8.213E-11	-4.784E-15	-1.20083E43	7.47283E0	DATA	51
3.349588E0	-2.6538E-45	4.8140E-6	-6.879E-09	2.6111E-12	-1.17971E46	2.42183E0	DATA	52
0.E0	0.E0	1.E0	1.E0				DATA	53
1000.00E0	28.0900E0	1.03944E0	SI	1			DATA	54
2.220792E01	1.74309E-3	-1.2008E-65	0.841E-10	-8.169E-14	-7.49661E2	-1.09166E1	DATA	55
4.245929E01	1.11866E-2	-1.9539E-51	6.109E-08	-4.991E-12	-4.80666E2	-2.75544E0	DATA	56
0.E0	0.E0	0.E0	1.E0				DATA	57
1000.00E0	12.000E0	2.32170E0	C	1			DATA	58
1.36325E001	1.85605E-3	-7.6675E-71	5.104E-10	-1.139E-14	-6.4967E02	-7.9890E00	DATA	59
-7.1244E-17	3.4065E-3	-5.5262E-6	1.514E-09	-2.382E-14	-6.80533E1	2.79326E0	DATA	60
1.E0	0.E0	0.E0	0.E0					

TABLE E-3. Typical Results From the Chemical Equilibrium Program

	FO/RT	INITIAL Y(I)
1 CH3	-0.2125516E 02	0.9999996E-01
2 CH4	-0.3390263E 02	0.9999996E-01
3 C2H	-0.1620010E 01	0.9999996E-01
4 C2H2	-0.1795241E 02	0.9999996E-01
5 H2	-0.1946587E 02	0.5000000E 00
6 H	-0.3306983E 01	0.1817857E 01
7 H2O	-0.4199399E 02	0.5000000E-01
8 OH	-0.2355809E 02	0.9999996E-01
9 CO	-0.3433722E 02	0.1781250E 01
10 CO2	-0.5534689E 02	0.9999996E-01
11 C2H4	-0.3240714E 02	0.9999997E-07
12 SiH	-0.5337708E 01	0.9999997E-07
13 SiH4	-0.3107219E 02	0.9999997E-07
14 SiO	-0.3503526E 02	0.5000000E-01
15 SiO2	-0.5489357E 02	0.5000000E-01
16 Si	-0.5333599E 01	0.1245673E 01
17 C	-0.2770977E 01	0.1819402E 01

NT = NO. ITERATIONS REQUIRED = 15      U=X/Y= 0.9999992

BB(J)= 4.30065060  
 BB(J)= 4.01785469  
 BB(J)= 2.28124809  
 BB(J)= 1.34567261

BETA = 0.1358E-03      TOTAL NO. OF MOLES= 7.6533      H= 0.0

FREE ENERGY F(Y) OF THE SYSTEM AT EQUILIBRIUM = -0.13351440E 03

PRESSURE= 0.10000E 01      TEMP = 0.20000E 04

I		Y(I)	MOLE FRACTION	MASS FRACTION
1	H2	0.2003845E 01	0.4668565E 00	0.5539759E-01
2	CO	0.1975098E 01	0.4601589E 00	0.7586706E 00
3	SIO	0.3060627E 00	0.7130653E-01	0.1850488E 00
4	H	0.4748080E-02	0.1106209E-02	0.6563182E-04
5	C2H2	0.1728777E-02	0.4027709E-03	0.6172804E-03
6	CH4	0.3832877E-03	0.8929848E-04	0.8432310E-04
7	SIH	0.1732134E-03	0.4035531E-04	0.6911633E-04
8	H2O	0.1095384E-03	0.2552029E-04	0.2706204E-04
9	CH3	0.3042049E-04	0.7087376E-05	0.6271996E-05
10	CO2	0.2365047E-04	0.5510093E-05	0.1427371E-04
11	C2H4	0.5377922E-05	0.1252949E-05	0.2068926E-05
12	C2H	0.3443769E-05	0.8023304E-06	0.1182037E-05
13	SIH4	0.1743203E-05	0.4061320E-06	0.7678682E-06
14	SIO2	0.1158856E-05	0.2699907E-06	0.9549212E-06
15	OH	0.2662728E-07	0.6203628E-08	0.6210342E-08
16	SI	0.1039440E 01	0.2421690E 00	0.4003937E 00
17	C	0.2321698E 01	0.5409100E 00	0.3820527E 00

		HEAT OF FORMATION	MASS FRACTION OF THE MIXTURE	ENTROPY
1	H2	0.0	0.3107945E-01	0.7275468E 02
2	CO	-0.2842813E 05	0.4256333E 00	0.7500009E 02

3	SIO	-0.2500515E 05	0.1038171E 00	0.7741382E 02
4	H	0.5422250E 05	0.3682109E-04	0.9031674E 02
5	C2H2	0.5257357E 05	0.3463100E-03	0.6054889E 02
6	CH4	-0.2164932E 05	0.4730739E-04	0.5537646E 02
7	SIH	0.8607963E 05	0.3877601E-04	0.8336095E 02
8	H2O	-0.6012953E 05	0.1518250E-04	0.7891264E 02
9	CH3	0.3051525E 05	0.3518747E-05	0.8537036E 02
10	CO2	-0.9484888E 05	0.8007915E-05	0.9794763E 02
11	C2H4	0.8626629E 04	0.1160720E-05	0.1168788E 03
12	C2H	0.1145694E 06	0.6631526E-06	0.9015688E 02
13	SIH4	0.5439773E 04	0.4307934E-06	0.1118265E 03
14	SIO2	-0.8350925E 05	0.5357354E-06	0.9616628E 02
15	OH	0.8756605E 04	0.3484164E-08	0.1174121E 03
16	SI	0.0	0.2246310E 00	0.1605104E 02
17	C	0.0	0.2143411E 00	0.9754942E 01

ENTHALPY OF GAS MIXTURE(CAL/GM-MOLE= 0.4021755E 03

MOLECULAR WEIGHT OF GAS MIX= 0.16989594E 02      ENTROPY( CAL/(GM-MOLE-OK) )= 0.436349E 01

## APPENDIX F

### METHOD FOR ESTIMATING PYROLYSIS PRODUCT COMPOSITION

#### Estimating the Pyrolysis Composition for a 40 Percent by Weight Nylon, 60 Percent by Weight Phenolic Resin

The most direct method of determining the products of degradation is the analysis by pyrolysis gas chromatography. This has been done by Sykes (1, 2) in which the hot degradation products were injected directly into the gas chromatograph. However, even with this procedure certain amount of condensation of heavy molecular weight species occur which remain unidentified and a possible source of error. The method has, however, reduced the total amount of unidentified material. Sykes has reported typical pyrolysis gas compositions for eighty-three percent of the total decomposition products evolved during the thermal degradation of nylon-phenolic resin composites (1, 2). The remaining seventeen percent was reported as an unidentified dark, tarry substance. This data is presented in Table F-1. The data of Friedman (5) for phenolic resin is presented in Table F-2 and there are fifteen percent unidentified materials. In addition, the data of Friedman (5) for nylon phenolic resin is presented in Table F-3. April (3) estimated a pyrolysis gas composition for his experimental work,

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TABLE F-1:      Pyrolysis product composition resulting  
                 from the degradation of a 40 percent  
                 nylon, 60 percent by weight phenolic  
                 resin, as reported by Sykes (2).

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<u>SPECIES</u>	<u>MASS FRACTION</u>
Phenol	0.118
Methylphenol	0.064
Dimethylphenol	0.051
Trimethylphenol	0.041
Benzene	0.003
Toluene	0.001
Cyclopentanone	0.029
Hydrogen	0.010
Methane	0.010
Carbon Monoxide	0.021
Carbon Dioxide	0.067
Water	0.062
Ammonia	0.002
Unidentified	0.173
Carbon Residue	0.340

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**TABLE F-3:**      Pyrolysis product composition resulting  
from the degradation of nylon phenolic  
resin, as reported by Friedman (5).

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<u>SPECIES:</u>	<u>MASS FRACTION</u>
Hydrogen	0.011
Methane	0.015
Ammonia	0.016
Water	0.064
Acetylene	0.066
Hydrogen Cyanide	0.022
Carbon Monoxide	0.071
Nitrogen	0.001
Ethylene	0.091
Ethane	0.001
Carbon Dioxide	0.023
Diacetylene	0.011
Acetone	0.010
Benzene	0.016
Toluene	0.011
Xylene	0.007
Isopropanol	0.018
Propane	0.015
Carbon Residue	0.529

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TABLE F-2      Pyrolysis product composition resulting  
from the degradation of phenolic resin,  
as reported by Friedman (5).

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<u>SPECIES</u>	<u>MASS FRACTION</u>
Carbon Dioxide	0.019
Carbon Monoxide	0.042
Benzene	0.004
Toluene	0.009
Phenol	0.181
Methylphenol	0.060
Methane	0.043
Water	0.114
Hydrogen	0.027
Unidentified	0.150
Carbon Residue	0.350

---



based on a comparison of the experimental and calculated heat of pyrolysis. His approach was, knowing the heat of pyrolysis, or heat of degradation, the heat of formation of these species and the reported analytically determined composition, estimate a new composition in such a way that the experimental and calculated values of the heat of pyrolysis agree within a few percent. His results are shown in Table F-4.

Since the compositions reported by Sykes (1, 2) and Friedman (5) have unidentified products and since the composition of April (3) does not agree with the elemental balance, a new composition based on the elemental balance constraints was arrived at in this research. The elemental composition for a 40 percent nylon, 60 percent by weight phenolic resin is shown in Table F-5. It is shown that for every 100 grams of polymer there are 73.80 grams of carbon, 7.36 grams of hydrogen, 3.95 grams of nitrogen and 14.89 grams of oxygen. The procedure is then to distribute the gram of these elements to each of the identified species in such a way that the elemental balance requirements are satisfied. A more detailed presentation is given by Hacker, et. al. (6).

#### Distribution of Oxygen Element

To accomplish the distribution of the oxygen element, an initial estimate based on the data of Table F-2 through Table F-4 is used. Table F-6 shows the initial estimate

---

**TABLE F-4:**      **Estimated pyrolysis gas composition of**  
**April (3).**

---

<u>SPECIES</u>	<u>MASS FRACTION</u>
Hydrogen	0.036
Water	0.478
Methane	0.058
Phenol	0.241
Carbon Monoxide	0.057
Dimethylphenol	0.087
Carbon Dioxide	0.025
Toluene	0.012
Benzene	0.006

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**TABLE F-5:**      Elemental composition of a 40 percent nylon,  
60 percent by weight phenolic resin  
composite.

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<u>ELEMENT</u>	<u>MOLES ELEMENT</u> <u>MOLE OF POLYMER</u>	<u>MASS ELEMENT</u> <u>100 GRAMS OF POLYMER</u>
C	8.19	73.80
H	9.87	7.36
N	0.376	3.95
O	1.240	14.89

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**TABLE F-6:** Initial and final estimates of the composition of the oxygen containing species.

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	INITIAL ESTIMATE	FINAL ESTIMATE
	(%)	(%)
Phenol	25	23.13
Water	7.5	7.20
Carbon Dioxide	5	4.61
Carbon Monoxide	5	4.66

---

and the adjusted final estimate which satisfies the elemental balance on oxygen. The dimethyl phenol, and trimethyl phenol were lumped into phenol for lack of thermodynamic data on these species. The total number of grams distributed among these species is 14.89.

#### Distribution of Hydrogen

The number of grams of hydrogen to be distributed among the hydrogen containing species is 7.36. However, only 4.80 grams are available since 2.86 grams were already distributed in phenol and water. The results of this distribution is shown in Table F-7.

#### Distribution of Nitrogen

The only nitrogen containing species is Nitrogen ( $N_2$ ) and the grams are 3.95 as shown in Table F-5.

#### Distribution of Carbon

The total grams of carbon available is 73.80. Of these, 34.50 have been distributed among some of the oxygen and hydrogen containing species, which are also carbon containing species. Hence, this leaves 39.30 grams of carbon which are to be assigned to the carbon species. The composition of all the species is presented in Table F-8.

---

**TABLE F-7:** Initial and final estimate of the composition of the hydrogen containing species.

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	INITIAL ESTIMATE	FINAL ESTIMATE
	(%)	(%)
Methane	3	3.87
Acetylene	3	3.89
Ethylene	3	3.89
Ethane	0.5	0.65
Benzene	2	2.58
Hydrogen	2	2.58

---

**TABLE F-8:** Estimate of the representative composition of the pyrolysis products for a 40 percent nylon, 60 percent by weight phenolic resin ablative composite.

Species	Mass Percent	Mole Percent
H <sub>2</sub>	2.57	20.92
CH <sub>4</sub>	3.86	3.90
C <sub>2</sub> H <sub>2</sub>	3.88	2.41
C <sub>2</sub> H <sub>4</sub>	3.88	2.24
C <sub>2</sub> H <sub>6</sub>	0.64	.35
C <sub>6</sub> H <sub>6</sub>	2.57	.53
C <sub>6</sub> H <sub>6</sub> OH	23.10	3.97
CO	4.65	2.40
CO <sub>2</sub>	4.60	1.69
H <sub>2</sub> O	7.29	6.45
N <sub>2</sub>	3.95	2.20
C(solid)	39.01	52.94

Element	Elemental Composition (mass percent)
C	73.80
H	7.36
O	3.95
N	14.89
Total	<u>100.00</u>

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1. Sykes, G. F., "Decomposition Characteristics of a Char Forming Phenolic Polymer Used for Ablative Composites", NASA IN-D-3810 (February 1967).
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6. Pike, R. W., G. C. April, E. G. del Valle, S. Hacker, "On Methods for Determining the Composition of Pyrolysis Products from Ablative Composites", Journal of Spacecraft and Rockets, 7, 1250-1253 (October 1970).



## APPENDIX G

### RESTRICTIVE EQUILIBRIUM ANALYSIS

In Chapter IV the equations for the chemical equilibrium analysis were developed. The analysis developed in Chapter IV consists of finding the equilibrium composition of a multicomponent, polyphase system by minimizing the free energy.

In reference (1) a method developed by del Valle and Pike was proposed whereby a restricted equilibrium state is defined. This equilibrium state is defined by adding to the free energy minimization algorithm an additional constraint; this constraint is in the nature of an energy balance constraint.

This constraint adds one extra equation to the free energy minimization technique. This technique was implemented at the suggestion of Swann from NASA (2). The reason for his suggestion was that at low temperatures the equilibrium composition of the degradation products of nylon-phenolic resins are not in agreement with experimentally determined values. In trying to improve the agreement the approach briefly described in this appendix was proposed. Therefore, it was developed for heuristic reasons and not for its theoretical value.

#### Heat Balance Constraint

The heat of pyrolysis of a degrading plastic can be

computed using the following equation (3):

$$\Delta H_{\text{pyr}} = \sum_{i=1}^q \{x_{p,i} \Delta H_{f,i} + \int_{298 \text{ K}}^{T_p} x_{p,i} C_{p,i} dT\} - \sum_{j=1}^l \{x_{r,j} \Delta H_{f,j} + \int_{298^\circ \text{K}}^{T_p} x_{r,j} C_{p,j} dT\} \quad (\text{G-1})$$

where the subscript p and r denote products and reactants respectively, q the total number of species present in the pyrolysis products and l the total number of components in the ablative composite. For nylon-phenolic resin composites, the temperature,  $T_r$ , where the degradation starts, is approximately  $300^\circ\text{C}$ , and the final temperature is approximately  $1000^\circ\text{C}$ . Pyrolysis products are generated over this temperature range and  $T_p$  is the appropriate average temperature which gives the correct energy associated with the pyrolysis products. It was determined to be  $700^\circ\text{C}$  as a weighted average based on the mass loss rate (3). Rearranging Equation G-1 gives,

$$\Delta H_{\text{pyr}} + \sum_{j=1}^l \{x_{r,j} \Delta H_{f,j} + \int_{298^\circ \text{K}}^{T_r} x_{r,j} C_{p,j} dT\} = - \sum_{i=1}^q \{x_{p,i} \Delta H_{f,i} + \int_{298^\circ \text{K}}^{T_p} x_{p,i} C_{p,i} dT\} \quad (\text{G-2})$$

The left hand side of Equation (G-2) is known from experimentally determined values. Lets define  $b_{m+1}$  as the left hand side, and let's drop the subscript p on the X's since we are going to deal only with the products.

$$b_{m+1} = \sum_{i=1}^q \{ x_i \Delta H_{f,i} + \int_{298^{\circ}\text{K}}^{T_p} x_i C_{p,i} dT \} \quad (\text{G-3})$$

Notice that the  $X_i$ 's are unknown. However, the right hand side of the equation which is unknown must satisfy the left hand side which is known. Equation (G-3) can be expanded to the form below:

$$b_{m+1} = \sum_{i=1}^n \{ x_i \Delta H_{f,i} + \int_{298^{\circ}\text{K}}^{T_p} x_i C_{p,i} dT \} +$$

$$\sum_{i=n+1}^1 \{ x_i \Delta H_{f,i} + \int_{298^{\circ}\text{K}}^{T_p} x_i C_{p,i} dT \} \quad (\text{G-4})$$

Note that Equation (G-4) has been written in the same form as the material balance expression shown in Equation (4-1). This simplified considerably the final form of the equations to be solved.

In addition, define  $H_i$  as:

$$H_i = \Delta H_{f,i} + \int_{298^{\circ}\text{K}}^T C_{p,i} dT$$

This is done to avoid carrying the integral term in the derivation; and the resulting equation is:

$$b_{m+1} = \sum_{i=1}^n H_i x_i + \sum_{i=n+1}^1 H_i x_i \quad (G-5)$$

### Lagrange Multiplier Formulation and Minimization

To form the augmented function, the additional constraint, Equation (G-5) is added to Equation (4-25) and this results:

$$G(X) = Q(X) + \sum_{j=1}^m \eta_j (b_j - \sum_{i=1}^1 a_{ij} x_i) +$$

$$\eta_{m+1} (b_{m+1} - \sum_{i=1}^1 x_i H_i)$$

Following a similar procedure to that developed in Chapter IV the resulting set of equations to be solved is as follows:

$$\sum_{j=1}^m r_{jk} \eta_j + b'_k u + \sum_{i=n+1}^1 a_{ij} x_i = b_k + \sum_{i=1}^n a_{ik} f_i(Y)$$

$$k=1 \dots m \quad (G-7)$$

$$\sum_{j=1}^m r_{jk} \eta_j + b'_k u + \sum_{i=n+1}^1 a_{ij} x_i = b_k + \sum_{i=1}^n a_{ik} f_i(Y)$$

$$k = m+1 \quad (G-8)$$

$$\sum_{j=1}^{m+1} b_j \eta_j = \sum_{i=1}^n f_i(Y) \quad (G-9)$$

$$\sum_{j=1}^{m+1} a_{ij} \eta_j = \left\{ \frac{F_0}{RT} \right\}_i \quad i=n+1 \dots l \quad (G-10)$$

It should be noted that Equations (G-7) and (G-8) have the same form. However, they are shown to emphasize the difference between the  $a_{ik}$ 's. The  $a_{ik}$ 's for  $k \leq m$  are the formula numbers as defined in Chapter IV. But  $a_{i,m+1} = H_i$ .

#### Comparison of Results Among Equilibrium, Restricted Equilibrium Analysis and Experimental Results

The chemical composition of the pyrolysis products resulting from the degradation of a 40 percent nylon, 60 percent phenolic resin ablative composite and computed by a restricted equilibrium analysis is presented in this section. The computations have been done for two decomposition temperatures because of the uncertainty involved in the properties to calculate the average temperatures. In addition two different energy constraints were used because of uncertainties in the heat of pyrolysis. The assumed average temperatures were 600° and 700°C and the energy constraints were -17,000 and -29,000 calories/gram-mole of polymer which correspond to -228 and -390 BTU/lb of composite. The results are presented in Table G-1 and Table G-2.

In Table G-1 a comparison of restrictive equilibrium with the experimental data of Sykes (4, 5) is given for two

TABLE G-1: Comparison of Restricted Equilibrium Analysis Compositions with the Experimental Data of Sykes (4,5) for a 40% Nylon, 60% Phenolic Resin Composite at a Temperature of 700°C and .1 atm.

Species	Restricted Equilibrium Mass Fraction for H = -29,999 cal/mole of polymer	Restricted Equilibrium Mass Fraction for H = -17,000 cal/mole of polymer	Experimental Mass Fraction
Phenol	10 <sup>-13</sup>	10 <sup>-13</sup>	0.118
Methyl Phenol	-	-	0.064
Dimethyl Phenol	-	-	0.051
Trimethyl Phenol	-	-	0.041
Benzene	10 <sup>-17</sup>	10 <sup>-17</sup>	0.003
Toluene	10 <sup>-13</sup>	10 <sup>-13</sup>	0.001
Cyclopentanone	-	-	0.029
Methane	0.025	0.024	0.010
Hydrogen	0.065	0.066	0.010
Carbon Monoxide	0.205	0.210	0.021
Carbon Dioxide	0.014	0.012	0.067
Water	0.021	0.019	0.062
NH <sub>3</sub>	10 <sup>-4</sup>	10 <sup>-4</sup>	0.002
N <sub>2</sub>	0.039	0.038	-
Unidentified	-	-	0.181
Carbon	0.631	0.630	0.350

energy constraints ( $H = -17,000$  and  $-29,000$  cal/mole of polymer) at a temperature of  $700^{\circ}\text{C}$ . The results show an order of magnitude agreement with the low molecular weight species identified by Sykes (4, 5). These are methane, hydrogen, carbon monoxide, carbon dioxide, water and ammonia. The agreement with the high molecular weight species, phenol, toluene, benzene, etc., was rather poor. The change in the energy constraint,  $H$ , from  $-17,000$  to  $-29,000$  cal/mole of polymer has different and opposite effects in several of the species. For example, an increase in the value of  $H$  had the effect of decreasing the amount of hydrogen, carbon and carbon monoxide, while increasing the concentrations of carbon dioxide and water. It should be noted that the mass fraction of unidentified species plus that of carbon makes up 0.521 of the total mass fraction of the experimental composition, while the restricted equilibrium predicts a mass fraction of 0.634 carbon. It should be further noticed that the mass of nitrogen makes up about four percent of the mixture. No nitrogen was reported in the experimental results (4, 5).

In Table G-2 a similar comparison is made, but the decomposition zone temperature is taken to be  $600^{\circ}\text{C}$ . Again an order of magnitude agreement is observed among the composition of the lower molecular weight species. Changing  $H$  affects the composition in the same fashion as was for the  $700^{\circ}\text{C}$  case.

TABLE G-2: Comparison of Restricted Equilibrium Analysis Compositions with the Experimental Data of Sykes (4,5) for a 40% Nylon, 60% Phenolic Resin Composite at a Temperature of 600°C and .1 atm.

Species	Restricted Equilibrium Mass Fraction for H = -29,000 cal/mole of polymer	Restricted Equilibrium Mass Fraction for H = -17,000 cal/mole of polymer	Experimental Mass Fraction
Phenol	10 <sup>-13</sup>	10 <sup>-13</sup>	0.118
Methyl Phenol	-	-	0.064
Dimethyl Phenol	-	-	0.051
Trimethyl Phenol	10 <sup>-13</sup>	10 <sup>-13</sup>	0.041
Benzene	10 <sup>-13</sup>	10 <sup>-13</sup>	0.003
Toluene	10 <sup>-13</sup>	10 <sup>-13</sup>	0.001
Cyclopentanone	-	-	0.029
Methane	0.039	0.036	0.010
Hydrogen	0.060	0.061	0.010
Carbon	0.160	0.167	0.021
Carbon Dioxide	0.027	0.024	0.067
Water	0.038	0.036	0.062
NH <sub>3</sub>	10 <sup>-4</sup>	10 <sup>-4</sup>	0.002
N <sub>2</sub>	.040	.040	-
Unidentified	-	-	0.181
Carbon	0.635	0.635	0.340
TOTAL	1.000	1.000	1.000



In general, restricted equilibrium provided an order of magnitude agreement for the composition of low molecular weight compound. It failed to give any agreement with the higher molecular weight component.

In table G-3 a comparison of restricted equilibrium with the general equilibrium analysis is given. It is shown that the compositions are within an order of magnitude of each other. The only mass fraction that is the same is that of nitrogen, since it is practically an inert, and that of carbon which agrees within one percent.

TABLE G-3: Comparison of Restricted Equilibrium Analysis With the General Equilibrium Analysis for a 40% Nylon, 60% Phenolic Resin Composite at 700°C and 1 atmosphere.

<u>Species</u>	<u>Restricted Equilibrium Mass Fraction for H = -29,000 cal/mole of polymer</u>	<u>Equilibrium Composition</u>
Phenol	$10^{-13}$	$10^{-18}$
Benzene	$10^{-17}$	$10^{-13}$
Toluene	$10^{-13}$	$10^{-13}$
Methane	0.025	0.043
Hydrogen	0.065	0.059
Carbon Monoxide	0.205	0.150
Carbon Dioxide	0.014	0.031
Water	0.021	0.043
NH <sub>3</sub>	$10^{-4}$	$10^{-4}$
N <sub>2</sub>	0.039	0.039
C	0.631	0.636

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## APPENDIX H

### EQUILIBRIUM CONVERSIONS OF CARBON-HYDROGEN- OXYGEN-NITROGEN REACTIONS

This appendix presents the equilibrium conversions at temperatures between 500°K and 3000°K for 100 chemical reactions in the C-H-O-N system.

The results presented in this appendix were used as a tool to help select the reactions of importance for the kinetics model. This is by no means an exhaustive search but it is indeed an extensive one.

Sources of these reactions were too many and varied to list them all. However, there were several sources that were extensive surveys of chemical reactions. One was a very specialized survey done by Pike (1) covering possible reactions resulting from the decomposition product of charring ablators. Another was an extensive Bibliography by Hockstein (2), and finally the work of Bahn (3). Bahn had a massive compendium of several hundred chemical reactions in the C-O-N system. Many of Bahn reactions were not analyzed because of the lack of available thermodynamic data.

The C-H-O-N system was divided into eight categories. These are carbon-hydrogen, carbon-oxygen, nitrogen-oxygen, hydrogen-oxygen, carbon-hydrogen-oxygen, carbon-hydrogen-nitrogen, hydrogen-nitrogen-oxygen and carbon-nitrogen-oxygen reactions.

A total of 47 reactions for the carbon-hydrogen reac-

tions are presented in Table H-1 with hydrocarbon reactions with up to four carbon atoms. Benzene and phenol reactions were not considered because the reactions for these components had already been selected and the kinetic data available was rather minimal.

Table H-2 presents seven carbon-oxygen reactions. Table H-3 lists 18 reactions in the nitrogen-oxygen system, except the last reaction in the table which is nitrogen dissociation. As can be seen,  $N_2$  is a pretty stable component even at the very high temperature of  $3000^{\circ}K$ . The same can be said about the dissociation of CO (reaction 5 in Table H-2).

Table H-4 is a compendium of 11 hydrogen-oxygen reactions. In contrast to the reactions of Tables H-1 through H-3, every reaction in this table has an equilibrium conversion greater than zero at  $3000^{\circ}K$ . It is interesting to note that reactions 1 and 3 have practically the same equilibrium conversion, at least to the number of significant digits shown; reaction 4 shows a very similar equilibrium conversion behavior as Equations 1 and 3. Reactions 9, 10, and 11 show the dissociation of hydroxyl radical, hydrogen and oxygen molecules respectively. As can be seen from the tabulation of the equilibrium conversion, there is no significant dissociation of these components until they reach a temperature of  $3000^{\circ}K$ .

Table H-5 lists 10 carbon-hydrogen-oxygen reactions. Except for the methylene radical reaction with CO, all other

**TABLE H-1: EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES  
FOR CARBON-HYDROGEN REACTIONS**

	<u>Equilibrium Conversion</u>			
	<u>500°K</u>	<u>1000°K</u>	<u>2000°K</u>	<u>3000°K</u>
1. $\text{CH}_4 = \text{CH}_3 + \text{H}$	0.	0.	0.94	48.01
2. $\text{CH}_4 = 1/2\text{C}_2\text{H}_6 + 1/2\text{H}_2$	0.	2.83	19.56	33.11
3. $\text{CH}_4 = 1/2\text{C}_2\text{H}_4 + \text{H}_2$	0.	5.05	91.27	98.71
4. $\text{CH}_4 = 1/2\text{C}_2\text{H}_2 + 3/2\text{H}_2$	0.	1.71	99.05	100.0
5. $\text{CH}_4 = \text{CH}_2 + \text{H}_2$	0.	0.	7.39	94.42
6. $\text{CH}_4 = \text{C}_{(\text{s})} + 2\text{H}_2$	3.0	84.77	99.92	100.00
7. $\text{CH}_3 = \text{CH}_2 + \text{H}$	0.	0.	1.27	49.37
8. $\text{CH}_2 = \text{CH} + \text{H}$	0.	0.	0.3	8.63
9. $\text{CH} = \text{C}_{(\text{g})} + \text{H}$	0.	0.	1.58	47.46
10. $\text{CH} = \text{C}_{(\text{s})} + \text{H}$	100.0	100.0	100.0	100.0

**TABLE H-1: EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES  
FOR CARBON-HYDROGEN REACTIONS (CONTINUED)**

	Equilibrium Conversion(5)			
	500°K	1000°K	2000°K	3000°K
11. $C_2H_6 = 2CH_3$	0.	0.	22.03	100.0
12. $C_2H_6 = C_2H_4 + H_2$	0.	50.52	99.99	100.0
13. $C_2H_6 = CH_4 + 1/2C_2H_4$	53.62	98.63	99.87	100.0
14. $C_2H_6 = CH_2 + CH_4$	0.	0.01	52.51	99.52
15. $C_2H_4 = C_2H_2 + H_2$	0.	4.51	99.77	100.0
16. $C_2H_4 = 2C + 2H_2$	100.0	100.0	100.0	100.0
17. $C_2H_2 = 2C + H_2$	100.0	100.0	99.96	99.21
18. $C_2H_2 = C_2H + H$	0.0	0.0	0.15	18.75
19. $C_2H = C_2 + H$	0.0	0.0	0.01	1.56
20. $C_2H_3 = C_2H_2 + H$	0.0	1.29	96.07	100.0

**TABLE H-1 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES  
FOR CARBON-HYDROGEN REACTIONS (CONTINUED)**

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
21. $C_3H_6 = C_2H_3 + CH_3$	0.	0.	11.37	98.31
22. $C_3H_6 = C_3H_5 + H$	0.	0.	72.37	100.0
23. $C_3H_5 = C_3H_4 + H$	0.	0.	2.07	30.88
24. $C_3H_4 = 3C + 2H_2$	100.0	100.0	100.0	100.0
25. $C_3H_8 = C_3H_6 + H_2$	0.01	87.15	100.0	100.0
26. $C_3H_8 = CH_4 + C_2H_4$	19.61	99.90	100.0	100.0
27. $C_6H_6 = 3C_2H_2$	0.	0.	99.48	100.0
28. $C_3H_6 + CH_3 = CH_4 + C_3H_5$	0.01	0.04	0.87	2.30
29. $CH_4 + C_4H_5 = CH_3 + C_4H_6$	0.0	0.42	5.69	12.66
30. $C_2H_4 + CH_4 = C_3H_6 + H_2$	0.38	6.63	24.34	25.27



TABLE H-1 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES  
FOR CARBON-HYDROGEN REACTIONS (CONTINUED)

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
31. $\text{CH}_3 + \text{H}_2 = \text{CH}_4 + \text{H}$	13.37	13.61	14.73	16.50
32. $\text{CH}_2 + \text{H} = \text{CH} + \text{H}_2$	0.	1.54	18.69	35.24
33. $\text{C}_{(\text{g})} + \text{H}_2 = \text{CH} + \text{H}$	0.	0.58	9.27	22.56
34. $\text{C}_{(\text{s})} + \text{H}_2 = \text{CH} + \text{H}$	0.	0.	0.	0.20
35. $\text{CH} + \text{C}_{(\text{s})} = \text{C}_2 + \text{H}$	0.	0.01	3.80	16.77
36. $\text{C}_2 + \text{H} = \text{CH} + \text{C}_{(\text{g})}$	0.	0.	0.15	1.81
37. $\text{C}_2\text{H} + \text{H} = \text{C}_2 + \text{H}$	0.	0.11	2.91	9.02
38. $\text{C}_2\text{H}_2 + \text{H}_2 = \text{C}_2\text{H}_3 + \text{H}$	0.	0.	0.04	0.75
39. $\text{C}_2\text{H}_2 + \text{H} = \text{C}_2\text{H} + \text{H}_2$	1.90	22.33	47.83	54.87
40. $\text{C}_2\text{H}_3 + \text{CH}_4 = \text{C}_2\text{H}_4 + \text{CH}_3$	33.37	33.38	33.55	45.55

TABLE H-1 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES  
FOR CARBON-HYDROGEN REACTIONS (CONTINUED)

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
41. $C_3H_5 + H_2 = C_3H_6 + H$	0.	0.	0.2	0.52
42. $I-C_4H_8 = 2C_2H_4$	0.29	93.90	100.0	100.0
43. $N-C_4H_{10} = C_3H_6 + CH_4$	69.67	100.0	100.0	100.0
44. $N-C_4H_{10} = 2C_2H_4 + H_2$	0.01	99.27	100.0	100.0
45. $N-C_4H_{10} = C_2H_6 + C_2H_4$	5.13	99.72	100.0	100.0
46. $I-C_4H_{10} = C_3H_6 + CH_4$	60.90	100.0	100.0	100.0

TABLE H-2: EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES  
FOR THE CARBON-OXYGEN REACTIONS

	Equilibrium Conversion			
	<u>500°K</u>	<u>1000°K</u>	<u>2000°K</u>	<u>3000°K</u>
1. $\text{C} + \text{O}_2 = \text{CO}_2$	100.	100.	100.	100.
2. $\text{C} + 1/2\text{O}_2 = \text{CO}$	100.	100.	100.	100.
3. $\text{CO}_2 = \text{CO} + \text{O}$	0.	0.	0.	19.0
4. $\text{C}_{(\text{s})} + \text{CO}_2 = 2\text{CO}$	0.	54.96	100.0	100.0
5. $\text{CO} = \text{C}_{(\text{g})} + \text{O}$	0.	0.	0.	0.
6. $\text{CO}_2 = \text{C}_{(\text{g})} + 2\text{O}$	0.	0.	0.	0.
7. $\text{CO}_2 + \text{O} = \text{CO} + \text{O}_2$	8.32	39.36	59.44	63.14

**TABLE H-3 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES  
FOR THE NITROGEN-OXYGEN REACTIONS**

	Equilibrium Conversion(%)			
	500°K	1000°K	2000°K	3000°K
1. $\text{NO} = \text{N} + \text{O}$	0.	0.	0.	0.04
2. $\text{N}_2 + \text{O}_2 = 2\text{NO}$	0.	0.	0.98	5.73
3. $2\text{NO} = \text{N}_2\text{O} + \text{O}$	0.	0.	0.03	1.50
4. $2\text{NO}_2 = 2\text{NO} + \text{O}_2$	4.91	93.99	99.79	100.0
5. $\text{N}_2\text{O} = \text{N}_2 + \text{O}$	0.	14.55	99.91	100.0
6. $\text{NO}_2 = \text{NO} + \text{O}$	0.	0.	39.26	99.47
7. $\text{N}_2\text{O} = \text{NO} + \text{N}$	0.	0.	3.81	100.0
8. $\text{NO} + \text{O}_2 = \text{NO}_2 + \text{O}$	0.	0.	0.02	1.18
9. $\text{NO} + \text{N} = \text{N}_2 + \text{O}$	0.	0.	0.01	0.4
10. $2\text{NO} = \text{NO}_2 + \text{N}$	0.	0.	0.	0.

TABLE H-3 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES  
FOR NITROGEN-OXYGEN REACTIONS (CONTINUED)

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
11. $\text{NO}_2 + \text{N}_2 = \text{NO} + \text{N}_2\text{O}$	0.	0.04	1.88	7.62
12. $\text{N}_2 + \text{O} = 2\text{N} + 1/2\text{O}_2$	0.	0.	0.	0.
13. $\text{N}_2 + \text{O}_2 = \text{NO}_2 + \text{N}$	0.	0.	0.	0.
14. $\text{NO} + \text{O} = \text{N} + \text{O}_2$	0.	0.	0.00	3.7
15. $\text{N}_2 + \text{O}_2 + \text{N}_2\text{O} + \text{O}$	0.	0.	0.	0.01
16. $\text{NO} + \text{N}_2 = \text{N}_2\text{O} + \text{N}$	0.	0.	0.	0.
17. $\text{N}_2\text{O} + \text{O}_2 = 2\text{NO} + \text{O}$	0.	0.	0.	0.
18. $\text{N}_2 = 2\text{N}$	0.	0.	0.	0.

**TABLE H-4 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES  
FOR THE HYDROGEN-OXYGEN REACTIONS**

	Equilibrium Conversion(%)			
	<u>500°K</u>	<u>1000°K</u>	<u>2000°K</u>	<u>3000°K</u>
1. $\text{H}_2\text{O} = \text{OH} + \text{H}$	0.01	2.20	15.94	27.33
2. $\text{H}_2\text{O} = \text{O} + \text{H}_2$	0.	0.	0.	7.19
3. $\text{H}_2\text{O} + \text{O} = 2\text{OH}$	0.	2.20	15.94	27.33
4. $\text{H}_2 + \text{O}_2 = 2\text{OH}$	0.03	2.26	16.79	27.93
5. $\text{O} + \text{H}_2 = \text{OH} + \text{H}$	37.06	48.31	54.25	56.29
6. $\text{O} + \text{OH} = \text{H}_2 + \text{OH}$	100.0	100.0	100.0	97.1
7. $\text{H}_2\text{O} + \text{H} = \text{H}_2 + \text{OH}$	0.37	4.57	24.26	36.87
8. $\text{H} + \text{O}_2 = \text{OH} + \text{O}$	0.18	6.11	32.73	47.96
9. $\text{OH} = \text{O} + \text{H}$	0.	0.	0.17	12.11
10. $\text{H}_2 = 2\text{H}$	0.	0.	0.01	7.82
11. $\text{O}_2 = 2\text{O}$	0.	0.	0.	5.71

TABLE H-5: EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES  
FOR THE CARBON-HYDROGEN-OXYGEN REACTIONS

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
1. $\text{CO}_2 + \text{H} = \text{CO} + \text{OH}$	0.	3.86	40.53	61.22
2. $\text{CH}_3 + \text{O}_2 = \text{CH} + 2\text{OH}$	0.	0.	2.24	65.59
3. $\text{CO}_2 + \text{H}_2 = \text{CO} + \text{H}_2\text{O}$	7.86	45.49	68.12	73.00
4. $\text{CH}_2 + \text{CO} = \text{C}_2\text{H}_2 + \text{O}$	0.	0.	0.02	0.23
5. $\text{C}_2\text{H} + \text{H}_2\text{O} = \text{C}_2\text{H}_2 + \text{OH}$	5.05	14.33	25.88	32.44
6. $\text{C}_2\text{H}_3 + \text{H}_2\text{O} = \text{C}_2\text{H}_4 + \text{OH}$	0.01	1.35	7.49	13.66
7. $\text{CH}_2 + \text{O} = \text{CO} + \text{H}_2$	100.	100.	100.	100.
8. $\text{CH}_4 + \text{O} = \text{CH}_3 + \text{OH}$	79.23	95.59	100.	100.
9. $\text{CH}_3 + \text{H}_2\text{O} = \text{CH}_4 + \text{OH}$	0.	0.71	5.24	10.36
10. $\text{C} + \text{H}_2\text{O} = \text{CO} + \text{H}_2$	0.	84.45	100.0	100.0

reactions show a measurable degree of conversion.

Table H-6, the last table of this appendix, is a compendium of carbon-hydrogen-oxygen, hydrogen-nitrogen-oxygen and carbon-nitrogen-oxygen reactions. A total of 8 reactions are presented in this table.



**TABLE H-6 : EQUILIBRIUM CONVERSION AT FOUR TEMPERATURES  
FOR THE CARBON-HYDROGEN-NITROGEN, HYDROGEN-  
NITROGEN-OXYGEN AND CARBON-NITROGEN-OXYGEN REACTIONS**

	Equilibrium Conversion			
	500°K	1000°K	2000°K	3000°K
1. $C + 1/2N_2 = C_2N_2$	0.	0.	0.	0.01
2. $HCN = H + CN$	0.	0.	0.	9.59
3. $NH_3 + C = HCN + H_2$	0.	12.12	99.92	100.0
4. $NH_3 = 1/2N_2 + 3/2H_2$	83.26	99.96	100.0	100.0
5. $N_2 + OH = N_2O + H$	0.	0.	0.0	0.1
6. $NO + OH = NO_2 + H$	0.	0.	0.36	1.20
7. $NO + CO_2 = NO_2 + CO$	0.	0.	0.21	1.88
8. $NO + CO = CO_2 + N$	0.	0.	0.06	1.86

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## VITA

Eduardo Gonzalez del Valle was born in [REDACTED], on [REDACTED]. He completed his primary and secondary education at the Jesuit run, Colegio de Belen, where he graduated June 16, 1960. Because of the communist take-over of Cuba, he was forced to leave his native country for the U. S. A. In the summer of 1960 he became Junior Counselor at Kingswood Camp, located in Pike, New Hampshire, which he had attended as a summer camper since 1956. The following year he became a Senior Counselor and was appointed instructor of swimming, boating and canoeing.

From September 1960 to June 1962, he attended Villanova University where he won for two consecutive years the Johnson Foundation Scholarship Award. Because of the family's financial difficulties, he moved to Miami where his parents lived. There he enrolled at the University of Miami for the school year 1962-1963, while working parttime. There he was awarded a diploma for "Outstanding Academic Achievement". In September 1963 he transferred to Louisiana State University where he received his Bachelor of Science Degree in Chemical Engineering in June 1965.

In his senior year, he received the Monsanto Chemical Company Scholarship Award.

As an undergraduate he was Editor of a Spanish newspaper called "Liborito". Also member and later Chairman of

a subcommittee of the Student Government Association. He became a member of the following honorary societies: Tau Beta Pi and Phi Kappa Phi.

On June 12, 1965, he married the former Margarita Garcia Du-Quesne. They have three children.

After graduation in 1965, he went to work for Kaiser Aluminum in Baton Rouge. The following year he started full time graduate work at LSU in February, 1966, and left in February, 1970. While in Graduate School he became member of the following honorary societies: Phi Lambda Upsilon and Sigma Xi.

In March 1970, he joined the Mathematics, Computer and Systems Department of Exxon Corporation in Florham Park, New Jersey. In August, 1973, he was transferred by Exxon to its refinery in Aruba, Netherlands Antilles, where he presently resides.

With his Dissertation, he will have a total of 24 publications.

## EXAMINATION AND THESIS REPORT

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Title of Thesis: In Depth Response of Ablative Composites

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